

09/787613  
UPDATED SEARCH  
SCAN

ENTRY SESSION  
0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 07:25:28 ON 12 DEC 2003  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 10 DEC 2003 HIGHEST RN 625425-12-9  
DICTIONARY FILE UPDATES: 10 DEC 2003 HIGHEST RN 625425-12-9

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s phenoxymethylbenzoic

L1 1 PHENOXYMETHYLBENZOIC

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN

RN 31719-75-2 REGISTRY

CN Benzoic acid, 3-(phenoxymethyl) - (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN m-Toluic acid, .alpha.-phenoxy- (7CI, 8CI)

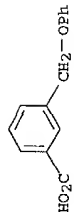
CN 3-Phenoxymethylbenzoic acid

FS 3D CONCORD

MF C14 H12 O3

LC STN Files:

USPATFULL BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER,  
(\*file contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s 'benzoic acid' and 'phenoxymethyl'

612623 "BENZOIC"

6181634 "ACID"

8404 "ACIDS"

6187878 "ACID"

("ACID" OR "ACIDS")

Connecting via Winsock to STN

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 SEP 09 CA/Caplus records now contain indexing from 1907 to the present

NEWS 4 AUG 05 New pricing for EUROPAFULL and FCITFULL effective August 1, 2003

NEWS 5 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN

NEWS 6 AUG 18 Data available for download as a PDF in RDISCLOSURE

NEWS 7 AUG 18 Simultaneous left and right truncation added to PASCAL

NEWS 8 AUG 18 PROPTI and KOSMET enhanced with Simultaneous Left and Right Truncation

NEWS 9 AUG 18 Simultaneous left and right truncation added to ANABSTR

NEWS 10 SEP 22 DIPPR file reloaded

NEWS 11 DEC 08 INPADOC: Legal Status data reloaded

NEWS 12 SEP 29 DISRAPs now available on STN

NEWS 13 OCT 10 PCTFULL: Two new display fields added

NEWS 14 OCT 21 BIOSIS file reloaded and enhanced

NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced

NEWS 16 NOV 24 MSDS-COOLS file reloaded

NEWS 17 DEC 08 CABA reloaded with left truncation

NEWS 18 DEC 08 IMS file names changed

NEWS 19 DEC 09 Experimental property data collected by CAS now available in REGISTRY

NEWS 20 DEC 09 STN Entry Date available for display in REGISTRY and CA/Caplus

NEWS EXPRESS NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01C. CURRENT

MACINTOSH VERSION IS V6.05(ENG) AND V6.05(JP)

AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003

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\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 07:25:20 ON 12 DEC 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL

611509 "BENZOIC ACID"  
L2 11954 "BENZOIC ACID" ("BENZOIC ACID")  
628 "BENZOIC ACID" AND "PHENOXYMETHYL"  
=> file caplus  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST  
SINCE FILE  
ENTRY  
18.96  
TOTAL  
SESSION  
19.17  
FILE 'CAPLUS' ENTERED AT 07:26:08 ON 12 DEC 2003  
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FILE COVERS 1907 - 12 Dec 2003 VOL 139 ISS 25  
FILE LAST UPDATED: 11 Dec 2003 (20031211/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2 and moisture content

237 L2  
161535 MOISTURE  
342 MOISTURES  
161620 MOISTURE  
(MOISTURE OR MOISTURES)  
1263004 CONTENT  
299978 CONTENTS  
1442509 CONTENT  
(CONTENT OR CONTENTS)  
39216 MOISTURE CONTENT  
(MOISTURE (W) CONTENT)  
0 L2 AND MOISTURE CONTENT

=> s l2 and moisture

237 L2  
161535 MOISTURE  
342 MOISTURES  
161620 MOISTURE  
(MOISTURE OR MOISTURES)  
1 L2 AND MOISTURE

=> d

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 20021504043 CAPLUS  
DN 137:48350  
TI Adhesive tapes for tape automated bonding (TAB) of semiconductor devices  
IN Yoshitaka, Ken; Aoki, Shoji; Shiozawa, Takashi  
PA Tomoe-gawa Paper Co., Ltd., Japan  
SO Jpn. Kokai Tokkyo Koho, 8 pp.  
CODEN: JKKXAF

DT Patent  
LA Japanese  
FAN CNT 1  
PATENT NO. KIND DATE APPLICATION NO. DATE  
PI JP 2002190502 A2 20020705 JP 2000-391345 20001222  
PRAI JP 2000-391345 20001222

=> s l2 and solvent

237 L2  
589327 SOLVENT  
294029 SOLVENTS  
743438 SOLVENT  
(SOLVENT OR SOLVENTS)  
14 L2 AND SOLVENT

=> d 1-14 ibib abs hitstr

L5 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
2003:673836 CAPLUS  
ACCESSION NUMBER:  
139:214121  
DOCUMENT NUMBER:  
TITLE:  
Preparation of ester group-containing ethers,  
sulfides, or amines  
Suzuki, Takashi; Kimura, Kazuhiko; Watanabe, Ryuzo  
Konica Co., Japan  
Jpn. Kokai Tokkyo Koho, 26 pp.  
SOURCE:  
CODEN: JKKXAF

DOCUMENT TYPE:

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

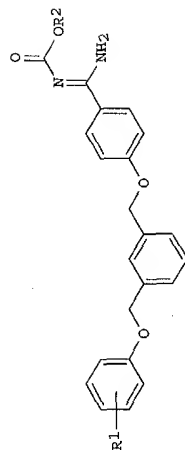
PATENT NO. KIND DATE APPLICATION NO. DATE

JP 2003238493 A2 20030827 JP 2002-33867 20020212  
PRIORITY APPLN. INFO.: JP 2002-33867 20020212  
OTHER SOURCE(S): MARPAT 139:214121  
AB R4Y(CR1R2)m(L1)PCO2R6 (I; R1, R2 = H, alkyl, cycloalkyl, aryl; R4 = alkyl, cycloalkyl, aryl, heterocyclyl; R6 = alkyl, cycloalkyl, aryl; Y = O, S, NR7; L1 = O, S, CO, SO2, NR8, alkylene, arylene; R7 = H, alkyl, cycloalkyl, aryl, heterocyclyl, sulfonyl; R8 = H, alkyl, cycloalkyl, aryl, heterocyclyl, acyl, sulfonyl, alkoxy, carbonyl, aryloxy, carbonyl, carbamoyl, sulfamoyl; m = 1-10; n = 0-10; R7 may be bonded to R4 forming a ring) are prepd. by reacting X(CR1R2)m(L1)PCO2R3 (II; R1, R2, L1, m, n = same as above; R3 = alkyl, cycloalkyl, aryl; X = halo) with R4YH (R4, Y = same as above) in R5OH (R5 = alkyl, cycloalkyl; R5 = noteq. R3). Use of R5OH which is different from alc. components of II, i.e. R5OH, reduces formation of carboxylic acids formed upon hydrolysis of products I. The reaction may be carried out in the presence of anhyd. metal salts capable of releasing water of crystn. upon heating. 2,5-BuO(tert-C8H17)C6H3SH was added to EtOH, mixed with Br(CH2)5CO2C8H17 at room temp., and the mixt. was heated under reflux for 3 h to give a product contg. 2,5-BuO(tert-C8H17)C6H3S(CH2)5CO2Et 6.1, 2,5-BuO(tert-C8H17)C6H3S(CH2)5CO2H (IV, impurity) 1.6%, vs. 88.3, and 2,5-BuO(tert-C8H17)C6H3S(CH2)5CO2H (IV, impurity) 1.6%, vs. 92.2% III and 3.6% IV for a control using octanol instead of EtOH as a solvent.

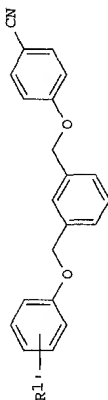
IT 56442-41-2P 124197-37-1P

RL: INF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(Prepn. of ester group-contg. (thio)ethers or amines from haloesters and alcs., thiols, or amines in alcs. different from alc. components of the esters)  
RN 56442-41-2 CAPLUS  
CN Benzoic acid, 4-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)

OTHER SOURCE(S):  
CI



I

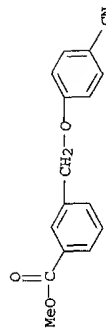


II

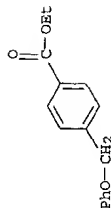
AB The title compds. II; C1-3 alkyl, cyclopentyl, cyclohexyl, Ph, PhCH2, (un)substituted C(CH3)2Ph; R2 = C1-3 alkyl, PhCH2] [e.g., Et [4-[3-[4-[1-(4-hydroxyphenyl)-1-methylethyl]phenoxy]methyl]benzyloxy]phenyl]iminomethyl]carbamate] are prepd. in high yield by the reaction of benzonitriles (II) in an arom. or ether solvent with lithium bis(trimethylsilyl)amide, sodium bis(trimethylsilyl)amide, or potassium bis(trimethylsilyl)amide, followed by reaction of the intermediate with carbonate ester halide R2O2CX (X = Cl, Br, OR2) followed by treatment with aq. HCl to give a hydrochloride salt of I.

IT 167569-28-0P, Methyl 3-(4-cyanophenoxy)methyl]benzoate  
RL: INF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(Procedure for the prodn. of aryl iminomethyl carbamic acid esters)

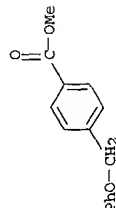
RN 167569-28-0 CAPLUS  
CN Benzoic acid, 3-[(4-cyanophenoxy)methyl]-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2000:277952 CAPLUS  
DOCUMENT NUMBER: 132:278989  
TITLE: Method for drying water- and/or solvent-wet 2-(phenoxy)methyl]benzoic acids  
INVENTOR(S): Isak, Heinz; Lambert, Martin  
PATENT ASSIGNEE(S): BASF A.-G., Germany  
SOURCE: PCT Int. Appl., 39 pp.



RN 124397-37-1 CAPLUS  
CN Benzoic acid, 4-(phenoxy)methyl]-, methyl ester (9CI) (CA INDEX NAME)

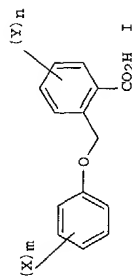


L5 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2001:523500 CAPLUS  
DOCUMENT NUMBER: 135:107153  
TITLE: Procedure for the production of aryl iminomethyl carbamic acid esters  
INVENTOR(S): Brandenburg, Joerg; Soyka, Rainer; Schmid, Rolf; Anderschewitz, Ralf; Bauer, Rolf; Ramm, Rainer; Kroeber, Jutta  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany  
SOURCE: Ger. Offen., 12 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

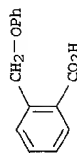
PATENT NO.	KIND DATE	APPLICATION NO.	DATE
DE 10000907	A1	20010719	20010719
US 2001009958	A1	20010726	20010726
US 6417382	R2	20020709	20010109
WO 2001051457	A2	20010719	20010719
WO 2001051457	A3	20020117	20010111
W: AE, AU, BG, BR, CA, CN, CZ, DE, HU, ID, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR			
BR 2001007551	A	20021008	20010111
EP 1250318	A2	20021023	20010111
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR			
JP 2003523328	T2	20030805	20010111
EE 200200392	A	20031015	20010111
US 2002137963	A1	20020926	20020505
NO 2002003348	A	20020711	20020711
BG 106916	A	20030430	20020712
PRIORITY APPLN. INFO.:			
DE 2000-10000907 A			20000112
US 2000-177378P P			20000124
US 2001-757253 A1			20010109

DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE  
 WO 2000023413 A1 20000427 WO 1999-EP7826 19991015  
 W: JP, US  
 RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
 DE 19848200 A1 20000427 DE 1998-19848200 19981020  
 EP 1123266 A1 20010816 EP 1999-950745 19991015  
 EP 1123266 B1 20030528  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI  
 JP 2002527499 T2 20020827 JP 2000-577141 19991015  
 AT 241363 E 20030615 AT 1999-950745 19991015  
 DE 1998-19848200 A 19981020  
 WO 1999-EP7826 W 19991015  
 OTHER SOURCE(S): MARPAT 132:278989  
 GI



AB 2-(Phenoxymethyl)benzoic acids (I; X, Y = halogen, C-org. radical; m = 0-5; n = 0-4) (e.g., 2-[(2-methylphenoxy)methyl]benzoic acid), wet with water and/or a solvent (e.g., methanol), are efficiently dried at 1-25.degree. above the i.m.p.  
 IT 724-98-1DP, 2-(Phenoxymethyl)benzoic acid, derivs.  
 RL: PUR (Purification or recovery); PREP (Preparation) (method for drying water- and/or solvent-wet 2-(phenoxymethyl)benzoic acids)  
 RN 724-98-1 CAPLUS  
 CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

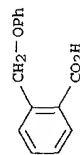
L5 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1997:702036 CAPLUS  
 DOCUMENT NUMBER: 127:358800  
 TITLE: Preparation of 6,11-dihydrodibenz(b,e)oxepin-11-ones  
 INVENTOR(S): Nishizawa, Susumu; Ueno, Hiroki  
 PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKKXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

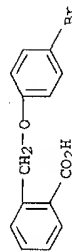
PATENT NO. KIND DATE APPLICATION NO. DATE  
 JP 09278774 A2 19971028 JP 1996-111952 19960408  
 PRIORITY APPLN. INFO.: JP 1996-111952 19960408  
 OTHER SOURCE(S): CASREACT 127:358800; MAREAT 127:358800  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Oxepinones I (R1 = H, Me; R2 = H, Cl-4 alkyl, OH, F, Cl, Br, nitrile, NO2, Cl-3 dialkylamino, Cl-4 alkoxy, etc.; R3 = H, F, Cl, Br, nitrile, NO2, Cl-4 alkyl, Cl-4 alkoxy, Cl-4 alkoxycarbonyl; n = 0-4) are prepd. by reaction of phenols I (R1, R2, n = same as I) with phthalides III (R3 = same as I) in the presence of MeONa at 150-180.degree., chlorination of IV (R1, R2, R3, n = same as I) with SOCl2 in PhNO2 in the presence of catalytic amt. of DMF, and without isolation of acid chlorides cyclocondensation with catalytic amt. of Lewis acids. 3-FC6C4OH was treated with phthalide in the presence of MeONa at 155-160.degree. for 4 h to give 78\* 2-(3-fluorophenoxymethyl)benzoic acid, which was chlorinated with SOCl2 in PhNO2 in the presence of DMF at 80.degree. for 2 h and cyclocondensed using AlCl3 at 20 degree. for 2 h to give 88\* 3-fluoro-6,11-dihydrodibenz(b,e)oxepin-11-one.  
 IT 724-98-1P, 2-Phenoxymethylbenzoic acid 728-96-1P  
 RL: IMF (Industrial manufacture); RCI (Reactant or reagent) (prepn. of dihydrodibenzoxepinones by ring opening of phthalides with phenols, chlorination, and cyclocondensation)  
 RN 724-98-1 CAPLUS  
 CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

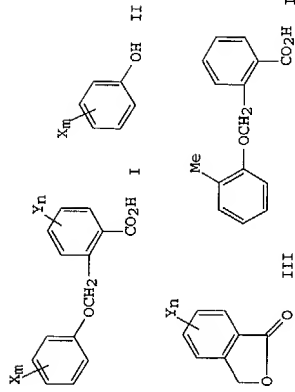


RN 728-96-1 CAPLUS  
 CN Benzoic acid, 2-[(4-bromophenoxy)methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1993:38276 CAPLUS  
 DOCUMENT NUMBER: 118:38276  
 TITLE: Open-chain nitrogen compounds. Part XV. A kinetic study of the hydrolysis of 1-aryl-3-[(aryloxy)methyl]-3-methyltriazenes and related triazenes  
 AUTHOR(S): Vaughan, Keith; Hooper, Donald L.; Merrin, Marcus P.





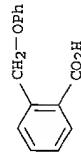
AB Title compds. (I: X, Y = halo, alkyl, alkoxy, CF<sub>3</sub>; m = 0-4; n = 0-3), were prepd. by a) conversion of phenol II to a phenolate by treatment with base, b) mixing the phenolate soln. with lactone III, c) distn. of solvent and heating of the resultant mixt. to 50-250.degree.. Thus, o-cresol was stirred with NaOMe in MeOH at 50.degree.; phthalide was added and solvent was distd. off. The residue was heated at 200.degree. to give 89% title compd. IV.

IT 724-98-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from phenol and phthalide)

RN 724-98-1 CAPLUS

CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1986:207175 CAPLUS  
 DOCUMENT NUMBER: 104:207175  
 TITLE: 6,11-Dihydrodibenz[b,e]oxepin-11-one  
 INVENTOR(S): Fuchs, Oskar; Nemes, Andras; Tolody, Lajos; Kasztreiner, Endre; Lazar, Arpad; Somogyi, Tibor; Balogh, Tibor  
 PATENT ASSIGNEE(S): Gyogyszerkutato Intezet, Hung.  
 SOURCE: Hung. Teljes, 9 pp.  
 CODEN: HUXXB  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Hungarian  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 34969	O	19850528	HU 1983-2142	19830616
HU 192812	B	19870728	HU 1983-2142	19830616

PRIORITY APPL. INFO.: CASREACT 104:207175  
 OTHER SOURCE(S):  
 AB 6,11-Dihydrodibenz[b,e]oxepin-11-one (I) is prepd. by the cyclization of

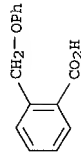
2-PhOCH<sub>2</sub>CH<sub>2</sub>COCl (II) (prepd. from the parent acid and SOCl<sub>2</sub>) in an arom. solvent at 60-120.degree. in the presence of Fe or alk. earth metal or oxide. Thus II (freshly prepd. from 6.84 kg the parent acid) in 20 L benzene was heated with 70 g freshly-reduced Fe to give 5.25 kg I. I is the starting material in the synthesis of doxepin.

IT 724-98-1

RL: PROC (Process)

RN 724-98-1 CAPLUS

CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1979:474309 CAPLUS

DOCUMENT NUMBER: 91:74309

TITLE: Studies on ketene and its derivatives. Part 89.

Ethyl 4-substituted acetoacetates: synthesis and reaction with diketene

Kato, Tetsuzo; Sato, Masayuki; Kimura, Hitochi

Pharm. Inst., Tohoku Univ., Sendai, Japan

Journal of the Chemical Society. Perkin Transactions

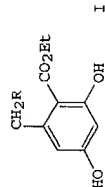
1: Organic and Bio-Organic Chemistry (1972-1999)

(1979), (2), 529-32

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English



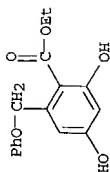
AB The benzoates I (R = Br, OEt, OPh, OCH<sub>2</sub>Ph, SPh, OAc) were prepd. (8-33%) by reaction of diketene with RCH<sub>2</sub>COCH<sub>2</sub>CO<sub>2</sub>Et (II). II (R = OEt, OPh, OCH<sub>2</sub>Ph, SPh, OAc) were obtained (44-70%) from II (R = Et) by reaction with NaR.

IT 71027-67-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 71027-67-3 CAPLUS

CN Benzoic acid, 2,4-dihydroxy-6-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1974:146640 CAPLUS  
 DOCUMENT NUMBER: 80:146640  
 TITLE: Synthesis of a copolymer from bis(p-carbomethoxy)phenoxyethylphosphinic acid, dimethyl terephthalate, or dimethyl sebacate and ethylene glycol

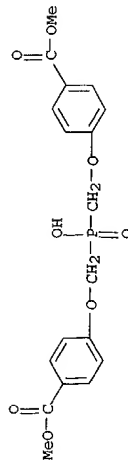
AUTHOR(S): Borisov, G.; Devedzhiev, I.  
 CORPORATE SOURCE: Inst. Org. Chem., Sofia, Bulg.  
 SOURCE: Izvestiya na Otdelenieto za Khimicheski Nauki (Bulgarska Akademiya na Naukite) (1972), 5(4), 553-9  
 CODEN: IOKNA5; ISSN: 0525-0889

DOCUMENT TYPE: Journal  
 LANGUAGE: Bulgarian  
 AB Bis[p-(methoxycarbonyl)phenoxyethyl]phosphinic acid (I) [47554-39-2] improved the thermal stability and fire resistance of poly(ethylene sebacate) [25034-96-2] and poly(ethylene terephthalate) [25038-59-9] copolymers. The polycondensation was carried out in the melt and the copolymers were sol. in basic solvents.  
 IT 51749-75-8 51749-76-9  
 RL: USES (Uses)

RN 51749-75-8 CAPLUS  
 CN Decanedioic acid, dimethyl ester, polymer with dimethyl 4,4'-(phosphinicobis(methyleneoxy))bis(benzoate) and 1,2-ethanediol (9CI)  
 (CA INDEX NAME)

CM 1

CRN 47554-39-2  
 CMF C18 H19 O8 P



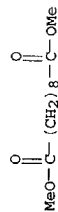
CM 2

CRN 107-21-1  
 CMF C2 H6 O2

HO-CH2-CH2-OH

CM 3

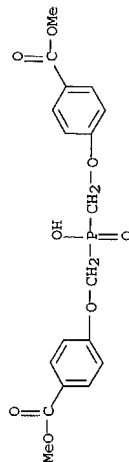
CRN 106-79-6  
 CMF C12 H22 O4



RN 51749-76-9 CAPLUS  
 CN 1,4-Benzenedicarboxylic acid, dimethyl ester, polymer with dimethyl 4,4'-(phosphinicobis(methyleneoxy))bis(benzoate) and 1,2-ethanediol (9CI)  
 (CA INDEX NAME)

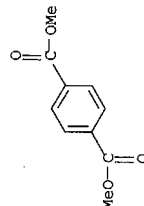
CM 1

CRN 47554-39-2  
 CMF C18 H19 O8 P



CM 2

CRN 120-61-6  
 CMF C10 H10 O4



CM 3

CRN 107-21-1  
 CMF C2 H6 O2

HO-CH2-CH2-OH

L5 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1973:44024 CAPLUS  
 DOCUMENT NUMBER: 78:44024  
 TITLE: Obtaining bis(p-carboxyphenoxyethyl)phosphinic acid, its esters, and polyesters

AUTHOR(S): Borisov, G.; Devedzhiev, I.  
 CORPORATE SOURCE: Inst. Org. Chem., Sofia, Bulg.  
 SOURCE: Doklady Bolgarskoi Akademii Nauk (1972), 25(6), 759-62

CODEN: DEANAD; ISSN: 0366-8681

DOCUMENT TYPE:

AB Bis(p-carboxyphenoxy)methylphosphinic acid (I) [37394-15-3] was

prepared by treatment of p-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me with Na and (ClCH<sub>2</sub>)<sub>2</sub>P(O)OH followed by sapon. with alc. K peroxide; I was copolymd. with each of 5 diols to give polyesters which were fire resistant and self-extinguishing. The polyesters had softening temps. sim. 300 deg., were insol. in ordinary org. solvents but sol. in org. and inorg. bases, and were capable of being drawn into fibers.

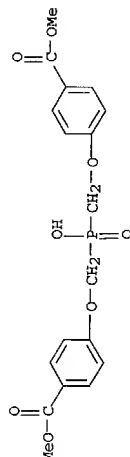
IT 47554-39-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

47554-39-2 CAPLUS

RN Benzoic acid, 4,4'-[bis(methyleneoxy)]bis-, dimethyl ester

CN (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

1971:105074 CAPLUS

DOCUMENT NUMBER:

74:105074

TITLE: Substituent effects in infrared spectroscopy. I. The O-H stretching frequencies in monomeric benzoic acids

EXPR, Otto; Svatek, E.

Cesk. Akad. Ved, Prague, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications

(1971), 36(2), 534-43

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE:

AB The O-H stretching frequencies of 60 meta- and para-substituted benzoic

acids were measured in dil. CCl<sub>4</sub> soln. The IR values were correlated by the Hammett equation with normal sigma consts. and slope rho = -11.7 cm<sup>-1</sup> on the one hand, and by the equation nu<sub>P=O</sub> = 1.14 (nu<sub>OH</sub>) on the other hand, where the frequency nu refers to the unsubstituted compd. The validity of the latter for substituents without an alpha. lone electron pair was confirmed even in IR spectroscopy. Somewhat lesser accuracy of the Hammett correlation is probably due to a different solvent than used in detg. the sigma consts.; deviations of a systematic character were not obsd.

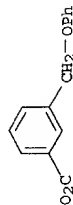
IT 31719-75-2 31719-76-3

RL: PRP (Properties)

(spectrum of, IR)

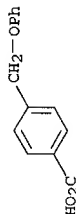
RN 31719-75-2 CAPLUS

CN Benzoic acid, 3-(phenoxy)methyl- (9CI) (CA INDEX NAME)



RN 31719-76-3 CAPLUS

CN Benzoic acid, 4-(phenoxy)methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

1970:121634 CAPLUS

DOCUMENT NUMBER:

72:121634

TITLE: Syntheses based on tetramethyloolphosphonium chloride. Some transformations of tris(chloromethyl)phosphine and methylbis(chloromethyl)phosphine oxide

TSvetkov, E. N.; Borisov, G.; Sivriev, Kh.;

Malevannaya, R. A.; Kabachnik, M. I.

SOURCE: Inst. Elementorg. Soedin., Moscow, USSR

Zhurnal Obshchei Khimii (1970), 40(2), 285-91

CODEN: ZOKH44; ISSN: 0044-460X

DOCUMENT TYPE:

AB Addn. of 350 g (HOCH<sub>2</sub>)<sub>4</sub>PCl to 1680 g PCl<sub>5</sub> in 2 l. CCl<sub>4</sub> at reflux and

heating 4 hr gave 97% (ClCH<sub>2</sub>)<sub>4</sub>PCl (I), m. 198-9 degree. I (200 g)

treated with 60.7 g NaOH in 300 ml H<sub>2</sub>O at 10-15 degree. in 400 ml H<sub>2</sub>O-400

ml CHCl<sub>3</sub> until alk. to phenolphthalein, gave 81.5% (ClCH<sub>2</sub>)<sub>3</sub>P (II), b<sub>2</sub>

56-7 degree. d<sub>20</sub> 1.4204, n<sub>D</sub> 20 1.5530, which on standing deposited a flaky

colorless solid of undetd. compn.; during evapn. of the solvent

from II the temp. must be held under 90 degree. as explosions occurred at

100 degree. or higher. II and 24% NaOH at 10-20 degree, then at reflux 3

hr until homogeneous gave MeP(O)(CH<sub>2</sub>Cl)<sub>2</sub> (III), b<sub>7</sub> 149-50 degree, m.

alone. Heated with NaOAc-AcOH 6 hr at 200 degree. III gave the diacetate,

b<sub>5</sub> 16 3-4 degree, 1.2326, 1.4670, also prepd. from II and AcOH-AcONa 10

hr at 150 degree. Heating II with EtSH-EtSNa 9 hr at 130 degree in Et<sub>2</sub>O

in an autoclave gave 84% (EtSCH<sub>2</sub>)<sub>3</sub>P, b<sub>2</sub> 137-8 degree, 1.0749, 1.5665.

MeP(O)(CH<sub>2</sub>Cl)<sub>2</sub> (IV) and Et<sub>2</sub>NH in 15 hr at 125 degree. gave 49% MeP(O)

(CH<sub>2</sub>NEt)<sub>2</sub>, b<sub>2</sub> cntdot. 5 118-19 degree, 0.9391, 1.4681. Heating 3 g IV

and 10 g Ph<sub>3</sub>P in Me<sub>2</sub>NCHO 12 hr at 150-60 degree. gave o n addn. of Me<sub>2</sub>CO

67.5% (Ph<sub>3</sub>PCl<sub>2</sub>)<sub>2</sub>P(O)Me<sub>2</sub>Cl-, m. 300-1.5 degree. IV (4 g) in MePh and a

refluxing 53.5% MeP(O)(CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub>, b<sub>5</sub> 185-6 degree, 1.1117, 1.4625.

Similarly was prepd. 52% MeP(O)(CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub>, b<sub>5</sub> 210-11.5 degree, 1.0082, 1.4547. Ph<sub>3</sub>PA similarly gave 83% MeP(O)(CH<sub>2</sub>OPh)<sub>2</sub>, m.

96-7 degree. Similarly was prepd. 80% p-tolyl analog, m. 122-4 degree.;

90-1 degree.; p-carbomethoxyphenyl analog, m. 133-5 degree.;

p-carboxyphenyl analog, m. 169-70 degree.; m-nitrophenyl analog, m.

26344-37-6P

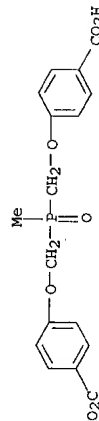
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

26344-37-6 CAPLUS

RN Benzoic acid, 4,4'-[(methylphosphinylidene)bis(methyleneoxy)]bis- (9CI)

CN (CA INDEX NAME)



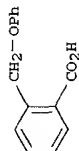


L5 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1966:4124 CAPLUS  
 DOCUMENT NUMBER: 64:4124  
 ORIGINAL REFERENCE NO.: 64:719c-e, 720a-b  
 TITLE: Dibenzo[b,e]oxepin-11-ones  
 INVENTOR(S): Bloom, B. M.; Tretter, J. R.  
 PATENT ASSIGNEE(S): Chas. Pfizer & Co. Inc.  
 SOURCE: 45 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

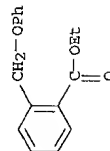
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 641498			BE	
GB 1018995		19640618	GB	

PRIORITY APPLIN. INFO.:  
 AB The title compds. (I) were prep'd. from the corresponding dibenzoxepin-11-one (II) and REINCH2CH2MgCl (III) and the resulting carbinol (IV) was dehydrated to I with mineral acids. Some salts of I were separated as salts of the cis and trans isomer by fractional crystn. The given synthesis affords a mixt. of 18% cis and 82% trans I. I are used as drugs in mental depression. The cis isomer is much more active than the trans one. omicron-BRCH2C6H4CO2Et (27.5 g.) is added to a soln. of 7.05 g. PhOH and 3 g. NaOH in 50 ml. H2O and the mixt. stirred at 100 degree. for 5 hrs. to give 10.22 g. Et 2-phenoxymethylbenzoate (V). 60.5-130-40 degree. V (10 g.) is added to a soln. of 100 ml. 10% 0.5 NaOH and 50 ml. EtOH and the mixt. refluxed 65 hrs. to give 8.9 g. 2-phenoxymethylbenzoic acid (VI), m. 125.5-26.5 degree. VI (15 g.) is added in 30 min. to 60 ml. (CF3CO)2O and the mixt. kept 4 hrs. at room temp. to give 10.5 g. II (X = Y = H), m. 70.5-1.5 degree. To a soln. of III (R = R1 = Me) in 200 ml. Et2O prep'd. from 11.5 g. MeNCH2CH2CH2Cl and 2.28 g. Mg, a 10% ethereal soln. of II (X = Y = H) is added in 1 hr. and the mixt. refluxed 20 hrs. to give 10 g. IV (X = Y = H, R = R1 = Me) (VII), m. 121-3 degree. VII (4.1 g.) in 100 ml. N HCl is refluxed 2 hrs. to give 3.08 g. I (X = Y = Me, R = R1 = Me), b.p. 260-70 degree.; HCl salt (VIIa) m. 188-9 degree. VII (10.4 g.) in 125 ml. C6H6 is added in 3 hrs. to a soln. of 6 g. BrCN in 50 ml. C6H6. After 30 min. the solvent is evap'd. at 15 mm. and 50 ml. C6H6 added to the residue; the soln. is washed with 50 ml. H2O, the solvent dist'd. 150 ml. 10% NaOH and 75 ml. EtOH are added to the residue, and the mixt. is refluxed 44 hrs. to give I (X = Y = H, R = R1 = Me) (VIII) as HCl salt, m. 241-2 degree. The following compds. are similarly prep'd.: II (X = H, Y = 2-MeNSO2), 11-allyl-dibenz[b,e]oxepin-11-ol, III.HCl (X = H, Y = 2-MeNSO2), R = H, R1 = Me), m. 199-201 degree.; II (X = H, Y = F3C), m. 108.5-9.5 degree. 168-9 degree. Several crystals. from EtOH give the trans salt, m. 172-3 degree. The cis hydrochloride m. 209-10.5 degree. Similarly is prep'd. cis-VIII.HCl, m. 225-6.5 degree., which with HCHO and HCO2H gives cis-VIIa.HCl. Heating 50 mg. trans-VIIa.HCl 0.25 hr. on a steam bath with 5 ml. N HCl gives a mixt. of the cis and trans isomers.

IT 724-98-1, o-Toluic acid, alpha-phenoxy-, ethyl ester (prepn. of)  
 RN 724-98-1 CAPLUS  
 CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



RN 4504-85-2 CAPLUS  
 CN Benzoic acid, 2-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)



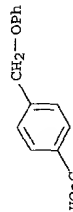
L5 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1963:32717 CAPLUS  
 DOCUMENT NUMBER: 58:32717  
 ORIGINAL REFERENCE NO.: 58:5468d-h, 5469a-b  
 TITLE: Quantitative evaluation of the inductive effect  
 AUTHOR(S): Exner, O.; Jonas, J.  
 CORPORATE SOURCE: Ustav Org. Chemie Csl. Akad. Ved. Prague  
 SOURCE: Collection of Czechoslovak Chemical Communications (1962), 27, 02298-306  
 CODEN: CCCCHK; ISSN: 0010-0765

DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The relative pK' values obtained by measuring the disson. consts. of p-toluic acids, substituted in the Me group, in 50% (by vol.) aq. EtOH (I) and 80% (by wt.) Methyl Cellosolve (II), are considered as a measure of the inductive effect of the substituents. From the results it follows that the transmission of the inductive effect takes place predominantly along the delta-bonds (and not space). Refluxing p-ClCH2C6H4CN (IIa) with azetropic HBr 12 hrs. gave 62% p-BrCH2C6H4CO2H, m. 229 degree. (EtOH), also formed in 90% yield by refluxing p-HOCH2C6H4CO2Me with the same reagent. p-ClCH2C6H4CO2H (III) (1-71 g.) and 4 g. NaI refluxed 1 hr. in 30 ml. Me2CO, the soln. evap'd. to dryness in vacuo, the inorg. salts washed out with H2O, and the product washed with a dil. soln. of Na2S2O3 gave 66% p-ICH2C6H4CO2H, m. 235 degree. (EtOH). Refluxing 1.71 g. III with 0.46 g. Na in 30 ml. abs. MeOH 3 hrs., evap'd. the MeOH in vacuo, and pptg. by HCl gave 70% p-MeOCH2C6H4CO2H, m. 108 degree. (CHCl3, petr. ether). Similar procedure with 1.71 g. III, 0.94 g. PhOH, and 0.46 g. Na in 30 ml. MeOH gave 55% p-PhOCH2C6H4CO2H, m. 216 degree. (dil. EtOH). Adding 0.8 ml. AcCl to 1.52 g. p-HOCH2C6H4CO2H in 5 ml. C5H5N, cooling the mixt. after 15 min., and pouring into dil. HCl gave 88% p-ACOCH2C6H4CO2H, m. 128 degree. (C6H6). p-PhCH2C6H4CO2H, prep'd. from p-BrCH2C6H4CN (IV) and C6H6 in a 68% overall yield, m. 160 degree. (dil. EtOH). Partial hydrolysis of p-NCH2C6H4CO2H afforded 51% p-H2NCOCH2C6H4CO2H, m. 274 degree. (EtOH). Refluxing 1.71 g. III with 1 g. NaSCN in 30 ml. EtOH 3 hrs., evap'd. the soln. to dryness in vacuo, eluting the salts with H2O, and reprecip. the crude product from 10% aq. KOH gave 60% p-NCSCH2C6H4CO2H, m. 172 degree. (EtOAc). Refluxing 1.61 g. p-BrCH2C6H4CO2H with 2.2 g. PhSO2Na in 25 ml. EtOH 8 hrs. yielded 95% p-PhSO2CH2C6H4CO2H, m. 306 degree. (decompn.) (EtOH). Adding 4.9 g. IV to a mixt. of 8.2 g. Me2NH.HCl and 3.5 g. NaOH in 10 ml. H2O and 25 ml. EtOH, allowing the mixt. to stand overnight, refluxing 30 min., evap'd. the EtOH in vacuo, dissolving the residue in H2O, extg. the soln. with three 15-ml. portions CHCl3, evap'd. the ext., refluxing the residue 3 hrs. with a soln. of 3 g. NaOH in 20 ml. 50% EtOH, acidifying the reaction mixt. with HCl,

evapd, to dryness in vacuo, and extg, the residue with boiling EtOH gave 56% p-Me2NCH2C6H4CO2H HCl, m. 256 degree. (EtOH) allowing a mixt. of 3.03 g. 1A and 2.8 g. (CH2)6N4 in 50 ml. CHCl3 to stand 2 days at room temp., concg. the soln. to 10 ml. in vacuo, filtering off 4.11 g. of a salt, and dissolving it in 20 ml. 1:2 HCl and EtOH, distg. to dryness in vacuo, and extg. the residue with Me2CO gave 52% p-H2NCH2C6H4CN.HCl, m. 269 degree. (EtOH). Hydrolysis by refluxing 16 hrs. with concd. HCl, followed by acetylation with AcCl in pyridine, gave 43% p-Ac-NHCH2C6H4CO2H, m. 201 degree. (EtOH). The measurements of the apparent disson. const. were carried out using an electronic pH meter with a vibrating condenser and a cell having a glass electrode and calomel reference electrode. The substances in concns. of the order of 10-3M were titrated with aq. Me4OH. The apparent disson. const. (pK') in solvents I and II for the appropriate substituents in .alpha.-position of p-MeC6H4CO2H are for: H, 5.78; 6.82; Cl, 5.36; 6.45; Br, 5.36; 6.36; iodine, 5.41; 6.41; Ph, 5.70; 6.73; CN, 5.28; 6.32; CONH2, 5.44; 6.69; OH, 5.56; 6.70; OMe, 5.50; 6.58; OPr, 5.43; 6.56; OAc, 5.46; 6.50; NHAc, 5.61; 6.68; NMe2.HCl, 4.67, ---; SCN, 5.33; 6.46; and PhSO2, ---, 6.36.

31719-76-3, p-toluic acid, .alpha.-Phenoxy- (ionization of)

IT 31719-76-3 CAPLUS (9CI) (CA INDEX NAME)



=> log hold  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST  
 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  
 CA SUBSCRIBER PRICE  
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 STN INTERNATIONAL SESSION SUSPENDED AT 07:30:08 ON 12 DEC 2003  
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 LOGINID:ssspal623zct  
 PASSWD:  
 \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
 SESSION RESUMED IN FILE 'CAPLUS' AT 08:22:34 ON 12 DEC 2003  
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 COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)  
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CA SUBSCRIBER PRICE  
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 L2 628 S "BENZOIC ACID" AND "PHENOXYMETHYL"  
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 L4 1 S L2 AND MOISTURE  
 L5 14 S L2 AND SOLVENT  
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 L6 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 DN 2000:277952 CAPLUS  
 TI 132:278989  
 IN Method for drying water- and/or solvent-wet 2-(phenoxyethyl)benzoic acids  
 IN Isak, Heinz; Lambert, Martin  
 PA BASF A.-G., Germany  
 SO PCT Int. Appl., 39 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 FAN.CNT 1  
 PATENT NO. KIND DATE APPLICATION NO. DATE  
 PI WO 2000023413 A1 20000427 WO 1999-EP7826 19991015  
 W: JP, US  
 RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
 DE 19848200 A1 20000427 DE 1998-19848200 19981020  
 EP 1123266 A1 20010816 EP 1999-950745 19991015  
 EP 1123266 B1 20030328  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI  
 JP 2002527499 T2 20030827 JP 2000-577141 19991015  
 AT 241583 E 20030615 AT 1999-950745 19991015  
 PRAI DE 1998-19848200 A 19981020  
 WO 1999-EP7826 W 19991015  
 OS MARPAT 132:278989  
 RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 L6 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 AN 1995:962988 CAPLUS  
 DN 124:146156  
 TI Preparation of oxime-containing heterocyclic compounds as agrochemical fungicides  
 IN Takase, Akira; Kai, Hiroyuki; Nishida, Kuniyoshi; Iwakawa, Tsuneo; Ueda, Kazuo; Masuko, Michio  
 PA Shionogi and Co., Ltd., Japan  
 SO PCT Int. Appl., 497 pp.

CODEN: PIXXD2					
DT Patent					
LA Japanese					
FAN.CNT 1					
PATENT NO. KIND DATE APPLICATION NO. DATE					
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	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BE, BU, CF, CG, CI, CM, GN, ML, MR, NE, SN, TD, TG				
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	CN 1094487	B	20021120		
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	US 6048885	A	20000411	US 1996-693224	19960821
	US 6268312	B1	20010731	US 1989-370255	19960809
	US 2002032227	A1	20020314	US 2000-728321	20001204
	US 6362212	B2	20020326		
	JP 1984-67819	A	19940401		
	WO 1995-JP604	W	19950330		
	US 1996-693224	A3	19960821		
	US 1999-370255	A3	19990809		
	MARPAT 124:146156				
OS	ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN				
L6	ANSWER 3 OF 9 CAPLUS				
AN	1993:233636	CAPLUS			
DN	118:233636				
TI	Orally active antiviral phenolic diethers				
IN	Girijavallabhan, Vijaykar M.; Ganguly, Ashit K.; Versace, Richard; Saksena, Anil K.; Pinto, Patrick A.				
PA	Schering Corp., USA				
SO	Eur. Pat. Appl., 41 PP.				
DT	CODEN: EPXXDW				
LA	English				
FAN.CNT 1					
PATENT NO. KIND DATE APPLICATION NO. DATE					
PI	EP 519702	A1	19921223	EP 1992-305551	19920617
	R: PT				
	CA 2111854	AA	19921223	CA 1992-2111854	19920617
	CA 2111854	C	20010109		
	WO 9222520	A1	19921223	WO 1992-US4961	19920617
	W: AU, BE, BG, BR, CA, CS, FI, HU, JP, KR, LK, MG, MW, NO, PL, RO, RU, SD, US				
	RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
	AU 9222213	A1	19930112	AU 1992-22213	19920617
	AU 674657	B2	19970109		
	ZA 9204445	A	19930224	ZA 1992-4445	19920617
	EP 590026	A1	19940406	EP 1992-913416	19920617
	EP 590026	B1	19950804		
	R: AT, BE, CH, DE, DK, ES, FR, GR, IE, IT, LI, LU, MC, NL, SE				
	JP 0650839	T2	19940428	JP 1992-501035	19920617
	PL 169699	B1	19960830	PL 1992-301825	19920617
	AT 182874	E	19990815	AT 1992-913416	19920617
	ES 2134808	T3	19991016	ES 1992-913416	19920617
	US 5350772	A	19940927	US 1993-39532	19930326

CODEN: PIXXD2					
DT Patent					
LA Japanese					
FAN.CNT 1					
PATENT NO. KIND DATE APPLICATION NO. DATE					
PI	WO 9526956	A1	19951012	WO 1995-JP604	19950330
	W: AM, AU, BE, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
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	CA 2186947	AA	19951012	CA 1995-2186947	19950330
	AU 9520843	A1	19951023	AU 1995-20843	19950330
	AU 865933	B2	19980129		
	EP 754684	A1	19970122	EP 1995-913382	19950330
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CN 1144524	A	19970305	CN 1995-192324	19950330
	CN 1094487	B	20021120		
	BR 9507203	A	19970909	BR 1995-7203	19950330
	US 6048885	A	20000411	US 1996-693224	19960821
	US 6268312	B1	20010731	US 1989-370255	19960809
	US 2002032227	A1	20020314	US 2000-728321	20001204
	US 6362212	B2	20020326		
	JP 1984-67819	A	19940401		
	WO 1995-JP604	W	19950330		
	US 1996-693224	A3	19960821		
	US 1999-370255	A3	19990809		
	MARPAT 124:146156				
OS	ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN				
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	CA 2111854	C	20010109		
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	AU 674657	B2	19970109		
	ZA 9204445	A	19930224	ZA 1992-4445	19920617
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	EP 590026	B1	19950804		
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	PL 169699	B1	19960830	PL 1992-301825	19920617
	AT 182874	E	19990815	AT 1992-913416	19920617
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	US 5350772	A	19940927	US 1993-39532	19930326

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	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BE, BU, CF, CG, CI, CM, GN, ML, MR, NE, SN, TD, TG				
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	AU 865933	B2	19980129		
	EP 754684	A1	19970122	EP 1995-913382	19950330
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	CN 1094487	B	20021120		
	BR 9507203	A	19970909	BR 1995-7203	19950330
	US 6048885	A	20000411	US 1996-693224	19960821
	US 6268312	B1	20010731	US 1989-370255	19960809
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	US 6362212	B2	20020326		
	JP 1984-67819	A	19940401		
	WO 1995-JP604	W	19950330		
	US 1996-693224	A3	19960821		
	US 1999-370255	A3	19990809		
	MARPAT 124:146156				
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SO	Eur. Pat. Appl., 41 PP.				
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	AU 674657	B2	19970109		
	ZA 9204445	A	19930224	ZA 1992-4445	19920617
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	R: AT, BE, CH, DE, DK, ES, FR, GR, IE, IT, LI, LU, MC, NL, SE				
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	PL 169699	B1	19960830	PL 1992-301825	19920617
	AT 182874	E	19990815	AT 1992-913416	19920617
	ES 2134808	T3	19991016	ES 1992-913416	19920617
	US 5350772	A	19940927	US 1993-39532	19930326

CODEN: PIXXD2					
DT Patent					
LA Japanese					
FAN.CNT 1					
PATENT NO. KIND DATE APPLICATION NO. DATE					
PI	WO 9526956	A1	19951012	WO 1995-JP604	19950330
	W: AM, AU, BE, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BE, BU, CF, CG, CI, CM, GN, ML, MR, NE, SN, TD, TG				
	CA 2186947	AA	19951012	CA 1995-2186947	19950330
	AU 9520843	A1	19951023	AU 1995-20843	19950330
	AU 865933	B2	19980129		
	EP 754684	A1	19970122	EP 1995-913382	19950330
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CN 1144524	A	19970305	CN 1995-192324	19950330
	CN 1094487	B	20021120		
	BR 9507203	A	19970909	BR 1995-7203	19950330
	US 6048885	A	20000411	US 1996-693224	19960821
	US 6268312	B1	20010731	US 1989-370255	19960809
	US 2002032227	A1	20020314	US 2000-728321	20001204
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	JP 1984-67819	A	19940401		
	WO 1995-JP604	W	19950330		
	US 1996-693224	A3	19960821		
	US 1999-370255	A3	19990809		
	MARPAT 124:146156				
OS	ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN				
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LA	Unavailable	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	BE 623259	19630405	BE			
	GB 950717		GB			
	NL 6508317		NL			
	NL 6508318		NL			
PRAI	DE 19611007					
L6	ANSWER 8 OF 9	CAPLUS	COPYRIGHT 2003	ACS	on STN	
AN	1963:33386	CAPLUS				
DN	58:33386					
OREF	58:5679a-g					
TI	Development of psychotropic compounds. I. New type ring systems					
AU	Stach, K.; Spingler, H.					
CS	C. F. Boehringer & Soehne G.m.b.H., Mannheim-Waldhof, Germany					
SO	Monatshefte fuer Chemie (1962), 93, 889-95					
CODEN:	MOCHM7; ISSN: 0026-9247					
DT	Journal					
LA	Unavailable					
L6	ANSWER 9 OF 9	CAPLUS	COPYRIGHT 2003	ACS	on STN	
AN	1959:6719	CAPLUS				
DN	52:6719					
OREF	52:1244d-f					
TI	Aromatic ether and thioether carboxylic acids					
PA	Henkel & Cie. G. m. b. H.					
DT	Patent					
LA	Unavailable					
PAN:	CNT 1					
PI	GB 773594	19570501	GB			

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L6 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 AB Na 2-hydroxymethylbenzoate (17.4 g.) and 9.4 g. phenol is heated with stirring in boiling xylene 6-8 hrs. to remove the H<sub>2</sub>O formed to give 11.5 g. 2-phenoxyethylbenzoic acid, converted to its ph ester, m. 69 degree., difficultly saponifiable with 40% NaOH, by successive reactions with PC15 and PhOH. Other omicron-benzoic acids and their esters prepd. are (omicron-ether group, m.p. or b.p., and ester group given): PhSCH<sub>2</sub>, m. 112 degree., n-octyl: BuOCH<sub>2</sub>, m. 63-4 degree., -; n-octyloxymethyl, m. 66-7 degree., -; 4-MeC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>, m. 124 degree., -; 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>OCH<sub>2</sub>, m. 104-5 degree., -; 4-tert-butylphenoxyethyl, m. 140 degree., -; bis[2-(2-phenoxyphenoxy)], m. 250 degree., -; xylenoxyethyl, b<sub>3</sub> 233-47 degree., n-octyl (b<sub>1</sub> 223-48 degree.), BuOCH<sub>2</sub>CH<sub>2</sub> (b<sub>1</sub> 224-44 degree.); 2-MeC<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>, m. 152 degree., 2-ethylhexyl (b<sub>1</sub> 221-4 degree.), benzyl (m. 42 degree. (alc.), b<sub>1</sub> 248-53 degree.); and S-2-carboxybenzylthioglycolic acid, m. 146 degree., -. The esters of the acids are useful as plasticizers.

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L6 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN  
 AB The synthesis of new ring systems was described. o-BrCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>COBr (139 g.) dissolved in 250 ml. abs. EtOH with stirring and cooling (ice H<sub>2</sub>O), the soln. treated dropwise with the appropriate Na phenolate or thiophenolate soln. (prepd. by adding 1 mole PhOH or PhSH or the appropriately

substituted derivs. of these 2 compds. to 23 g. Na dissolved in 500 ml. abs. EtOH at room temp. with stirring, the whole boiled 2-3 hrs., cooled, the ppt. filtered off, washed with EtOH, the combined filtrate and washings concd. to 1/3 its vol., treated with H<sub>2</sub>O, the Et<sub>2</sub>O layer sep'd., washed with 5% aq. NaOH and H<sub>2</sub>O, dried, evapd., the residue boiled 2-3 hrs. with 500-600 ml. MeOH contg. 50-60 g. KOH, the soln. evapd. in vacuo on a water bath, and the residue treated with H<sub>2</sub>O and Et<sub>2</sub>O, the aq. layer sep'd., filtered, and the filtrate acidified with 6N HCl gave the following 2-(RC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H (I) (S, Z, b.p./mm., m.p., % yield given): H, O, 155-8 degree., div. 0.03, 125-6 degree., 69.0; 4-Me, O, 162-7 degree., div. 0.05, 126-9 degree., 71.0; 4-MeO, O, 190-5 degree., div. 0.1, 176-8 degree., 78.0; 4-Br, O, 190-2 degree., div. 0.03, 182-4 degree., 67.0; 3-Me, O, -, 145-8 degree., 77.0; H, S, 167-72 degree., div. 0.15, 109-12 degree., 84.0; 4-Me, S, 173-8 degree., div. 0.05, 128-30 degree., 85.0; 4-MeO, S, 184-90 degree., div. 0.1, 116-19 degree., 82.0; 4-Cl, S, 168-72 degree., div. 0.05, 128-8 degree., 88.0. Method A. P205 (21.0 g.) added portionwise to 14 ml. abs. EtOH initially at room temp. and towards the end at 50-80 degree. (internal temp.), the mixt. heated 1 hr. at 95-100 degree. until the P205 had completely reacted, treated with 0.05 mole I (Z = O) at 80-90 degree., heated 30 min. at a definite temp. range, added while hot (80 degree.) to ice H<sub>2</sub>O with stirring, the product isolated with Et<sub>2</sub>O, distd. in vacuo, and the distillate treated with ligroine or ligroine-Et<sub>2</sub>O or recrystd. from iso-PrOH gave the following II (Z = O) [R, reaction temp., b.p./mm., % yield, m.p. (log member.) in MeOH and isooctane, resp., nu. (KBr) (cm.<sup>-1</sup>) given]: H, 100-10 degree., 142-5 degree., div. 0.2, 85.5; 71-2 degree., 267.9 (4.18) and 263.3 (4.21), 1651; 2-Me, 100-10 degree., 147-50 degree., div. 0.1, 82.0, 108-9 degree., 268.9 (4.22) and 265.3 (4.23), 1648; 2-MeO, 130-40 degree., 158-62 degree., div. 0.05, 81.0, 93.4 degree., 271.0 (4.17) and 265.6 (4.15), 1644; 2-Cl, 130-40 degree., 162-6 degree., div. 0.5, 71.5, 126-7 degree., 266.8 (4.19) and 263.6 (4.24), 1649; 3-Me, 100-10 degree., 140-7 degree., div. 0.1, 54.0, 71-2 degree. (ligroine-Et<sub>2</sub>O), 275.0 (4.24) and 270.3 (4.21), 1648. Method B. I (Z = O) (0.025 mole) and 6 ml. SOCl<sub>2</sub> boiled 1 hr., the excess SOCl<sub>2</sub> removed in vacuo, the residue heated at a definite temp. range (oil bath) while introducing a stream of dry N until the end of evolution of HCl (1-2 hrs.), the product distd. in vacuo, and the distillate further purified as in method A gave the following II (Z = O) (identical b.ps. and m.ps. as in method A) [R, reaction temp., and % yield given]: H, 150-60 degree., 71.0; 2-Me, 130-40 degree., 88.5; 2-MeO, 200-20 degree., 42.5; 2-Cl, 150-60 degree., 78.0; 2-Br [b<sub>0</sub>0.5 C. I (Z = S) (0.1 mole) added to 140 g. polyphosphoric acid at 80 degree. with stirring, the mixt. heated 30 min. at a definite range, added while hot (80 degree.) to ice H<sub>2</sub>O with stirring, the product isolated with Et<sub>2</sub>O or CH<sub>2</sub>Cl<sub>2</sub>, distd. in vacuo, and the distillate further purified as in method A gave the following II (Z = S) [R, reaction temp., b.p./mm., % yield, m.p. (iso-PrOH), lambda. (max. of the conjugated band) (nu. (KBr) (cm.<sup>-1</sup>) log member.) in MeOH and isooctane, resp., nu. (KBr) (cm.<sup>-1</sup>) given]: H, 100-10 degree., 162-5 degree., div. 0.03, 84.5, 86-8 degree., 242.0 (4.34) and 241.4 (4.37), 1651; 2-Me, 100-10 degree., 167-75 degree., div. 0.2, 86.5, 119-20 degree., 242.3 (4.37) and 240.6 (4.44), 1633; 2-Cl, 130-40 degree., 175-81 degree., div. 0.2, 81.0, 133-4 degree., 243.2 (4.38) and - (difficultly sol. in isooctane), 1660. 2-Ph-(CH<sub>2</sub>)<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H (0.1 mole) treated according to method C (30 min. at 150-60 degree.) gave 66.0% III, b<sub>0</sub>1 150-3 degree., m. 147-8 degree. (iso-PrOH), lambda. (max. of the conjugated band) (MeOH) 263.0 m.mu. (log member. 4.18), nu. (KBr) 1633 cm.<sup>-1</sup>.

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For diagram(s), see printed CA Issue.

Dibenz[b]elalkylideneoxepines and thiepinones were prepd. by treating under Grignard conditions 0.05 mole dibenz[b]eloxepin- (I) or dibenz[b]thiepin-11-one (II) with an aminoalkylmagnesium iodide (from 1.82 g. Mg and 0.075 mole aminoalkyl iodide) to form an 11-hydroxy-11-(aminoalkyl)dibenz[b]eloxepine or dibenz[b]elthiepine, and heating 0.02 mole of the product with 25ml. 7-8N HCl in EtOH. The following III (X = O) (IV) and V (X = O) (VI) were prepd. [R, R<sub>1</sub>, m.p. III (X = O), and m.p. IV, HCl (X = O) given]: Me<sub>2</sub>N, H, 118-19 degree.; [maleate salt 161-4 degree.]; Me<sub>2</sub>N, Me, 125-7 degree., 176-8 degree.; Me<sub>2</sub>N, Cl, 107-11 degree., 183-5 degree. (tetrahydrate); Me<sub>2</sub>N, Cl, 140-4 degree., 216-18 degree.; piperidino, H, 140-3 degree., [succinate salt m. 136-8 degree.]; N'-methyl-N-piperazinyl, H, 151-5 degree., decomp. 256-8 degree. (dihydrate); PhCH<sub>2</sub>Me, H, 104-7 degree., [b.o. 1220-30 degree.]. The following III (X = S) (VII) and V (X = S) (VIII) were prepd. [R, R<sub>1</sub>, m.p. VII, and m.p. VIII given]: Me<sub>2</sub>N, H, 130-2 degree., 216-18 degree.; Me<sub>2</sub>N, Me, 133-7 degree., 206-8 degree.; Me<sub>2</sub>N, Cl, 133-7, 2346 degree. (tetrahydrate); piperidino, H, 181-3 degree., 250-1 degree. (dihydrate); and PhCH<sub>2</sub>Me, H, 108-9 degree., b.o. 15 210-25 degree. VI (R = Me<sub>2</sub>N, R<sub>1</sub> = H), VIII (R = Me<sub>2</sub>N, R<sub>1</sub> = H), VII (R = Me<sub>2</sub>N, R<sub>1</sub> = Cl), and 11-3-(N'-methyl-N-piperazinyl)propylidenedibenz[b,e]thiepine-HCl, m. 255-7 degree., were prepd. in a one stage process. I, m. 71-2 degree., was prepd. in 85.5% yield by adding portionwise 129 g. P<sub>2</sub>O<sub>5</sub> to 85 ml. EtOH with cooling (50-80 degree.), heating the mixt. 1 hr. at 95-100 degree., adding at 90 degree. 88.4 g. o-phenoxymethylbenzoic acid (IX) in 2 portions, heating the mixt. 15 min. at 100 degree. after the first addn. and 30 min. after the second, pouring the mixt. onto ice and extg. with EtO. Similarly were prepd. the following derivs. (substituent given): 2-Me (X), m. 108-9 degree. (iso-PrOH); 2-MeO (XI), m. 93-4 degree.; 2-Cl (XII), m. 126-7 degree.; and 3-Me, m. 71-2 degree., with polyphosphoric acid or H<sub>3</sub>PO<sub>4</sub> and P<sub>2</sub>O<sub>5</sub> as dehydrating agents. II, m. 88-9 degree., and its 2-Me, m. 119-20 degree.; 2-Cl, m. 130-2 degree.; and 2-MeO, m. 89-90 degree. IX, m. 125-6 degree., was prepd. in 69% yield by dissolving 367.5 g. o-BrC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>Br in 660 ml. abs. EtOH at 10 degree., adding dropwise to the mixt. at room temp. a soln. prepd. from 62 g. Na, 1320 ml. EtOH, and 250 g. PhOH, refluxing the mixt. 2 hrs., filtering and evapg. the filtrate, decompg. the residue with H<sub>2</sub>O and Et<sub>2</sub>O, sepg., washing, and evapg. the Et<sub>2</sub>O ext., refluxing the residue 2 hrs. with 130 g. KOH and 1200 ml. MeOH, evapg., extg. the residue with H<sub>2</sub>O and Et<sub>2</sub>O, and acidifying the aq. ext. Similarly were prepd. the following o/p-(R-substituted) phenoxymethylbenzoic acids (R and m. p. given): Me, 118-20 degree.; MeO, 176-8 degree.; and Cl, 162-4 degree.. o-(m-Methylphenoxymethyl)benzoic acid m. 145-8 degree.. The following o/p-[R-substituted] phenylthiomethyl benzoic acids were prepd. R and m.p. given: H, 106-9 degree.; Cl, 125-8 degree.; Me, 128-31 degree.; and MeO, 116-19 degree. I was also prepd. in 61% yield by heating under N 5 g. o-phenoxymethylbenzoyl chloride (XIII) 2.5 hrs. at 100-10 then 0.5 hrs. at 150-60 degree. and distg. in vacuo. Alternatively I was prepd. by heating 5 g. XI 5 hrs. in 5 ml. xylene, or by heating 11.4 g. IX 8 hrs. in 12 ml. xylene with 4.5 ml. SOCl<sub>2</sub>; or, preferably, by refluxing 5.7 g. IX 2 hrs. with 5 ml. SOCl<sub>2</sub>, removing excess SOCl<sub>2</sub>, and heating the residue approx. 2 hrs. under N at 150-60 degree.; or by adding 6.7 g. AlCl<sub>3</sub> to 12.3 g. XIII in 45 ml. CS<sub>2</sub> and 10 ml. PhNO<sub>2</sub>, keeping the mixt. 5 hrs. at room temp., refluxing 1 hr., pouring the mixt. on ice, and washing the org. ext. with 2% NaHCO<sub>3</sub> s<sup>s</sup>, NaOH, and H<sub>2</sub>O, and evapg. in vacuo. Similarly were prepd. X, XII, and 2-bromodibenz[b]eloxepin-11-one, m. 135-7 degree. (iso-PrOH); XII, m. 48-51, was prepd. in 93% yield by refluxing 3 hrs. 45.6 g. IX and 73 ml. SOCl<sub>2</sub>, evapg. the mixt. in vacuo, and recrystg. from MeOH, or by adding dropwise at 20-5 degree. 7 ml. SOCl<sub>2</sub> in 10 ml. CHCl<sub>3</sub> to 10.6 g. IX in 25 ml. CHCl<sub>3</sub> and refluxing 8 hrs. The title compds. are tranquilizers.

=> d abs 5-6

ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

For diagram(s), see printed CA Issue.

Reaction between acetanilides and aryl glycidyl ethers using tertiary amines as catalysts gave 2-oxazolidone derivs. if an electron-withdrawing group, CCl<sub>3</sub> or CF<sub>3</sub> is present in the acid component of the acid amide. Me, Ph, or p-ClC<sub>6</sub>H<sub>4</sub> groups in the acid component of the acid amide gave N-(3-phenoxy-2-hydroxypropyl)aniline (I) and N,N-bis(3-phenoxy-2-hydroxypropyl)aniline (II). These results suggest that the nucleophilic attack of the imide group of the acid amide on the epoxy ring occurred easily but when the acid component of the acid amide is a Me group the acyl reaction gave I since C-C bond scission was difficult. PhCOCl (13.3 g.) in 60 ml. Me<sub>2</sub>CO was added with stirring at -10 degree. to a soln. of 9.3 g. p-EOC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> and 10.1 g. Et<sub>3</sub>N in 100 ml. Me<sub>2</sub>CO and the mixt. was kept 1 hr. at room temp. to give 72% alpha., alpha., alpha.-trifluoro-p-ethoxyacetanilide m. 139-40 degree.. Similarly were prepd. the following RNHCOR' (R, R', and m.p. given): Ph, CCl<sub>3</sub>, 91-3 degree.; p-MeC<sub>6</sub>H<sub>4</sub>, CCl<sub>3</sub>, 110.5-11.5 degree.; p-EtOC<sub>6</sub>H<sub>4</sub>, CCl<sub>3</sub>, 124-6 degree.; p-ClC<sub>6</sub>H<sub>4</sub>, CCl<sub>3</sub>, 124.5-5.5 degree.; p-MeOC<sub>6</sub>H<sub>4</sub>, CCl<sub>3</sub>, 115-18 degree.; Ph, PhN,N-NC<sub>6</sub>H<sub>4</sub>, CCl<sub>3</sub>, 143-5 degree.; Ph, CF<sub>3</sub>, 88-9 degree.; p-MeC<sub>6</sub>H<sub>4</sub>, CF<sub>3</sub>, 109-11 degree.; p-ClC<sub>6</sub>H<sub>4</sub>, CF<sub>3</sub>, 122-3 degree.; o-MeC<sub>6</sub>H<sub>4</sub>, CF<sub>3</sub>, 79-80 degree.; Ph, Me, 113-14 degree.; Ph, Ph, 131-2 degree.; Ph, ClCH<sub>2</sub>, p-ClC<sub>6</sub>H<sub>4</sub>, 116-17 degree.; Ph, PhCH<sub>2</sub>, 91-3 degree.; Ph, CCl<sub>3</sub>, 193-4 degree. (?); Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 179-80 degree.; Ph, NCC<sub>6</sub>H<sub>4</sub>, 205-6 degree.; Ph, HCF<sub>2</sub>CF<sub>2</sub>, 66-8 degree.; Ph, NCC<sub>6</sub>H<sub>4</sub>, 194-5 degree.; NaOMe (54 g.) in 400 ml. MeOH was added to a mixt. of 128.5 g. p-chlorophenol and 370 g. epichlorohydrin with stirring during 1 hr. at room temp. and the mixt. stirred an addnl. hr. to give 78% p-chlorophenyl glycidyl ether, b2 115-16 degree., n<sub>D</sub>20 1.5419. Triethylenediamine (0.1 g.) was added to a mixt. of 13.5 g. acetanilide and 15 g. phenyl glycidyl ether, heated to 100 degree. to soln., then heated 2 hrs. at 100 degree., cooled, and poured into a soln. of 100 g. Ac<sub>2</sub>O in 80 g. pyridine and kept overnight at room temp. to give 9.5 g. II diacetate and 9.8 g. I diacetate. Phenyl glycidyl ether (4.5 g.) was added to 9.5 g. PhNH<sub>2</sub> at 120 degree. over 1 hr. and kept an addnl. 15 min. to give 80.9% I, m. 60-2 degree.. I was acetylated by pyridine and Ac<sub>2</sub>O to give the diacetate, m. 96-7 degree.. Phenyl glycidyl ether (4.5 g.) in 50 ml. benzene was added to a boiling soln. 6.5 g. I in 30 ml. benzene, the mixt. refluxed 1 hr., benzene removed, and the residue dissolved in pyridine-Ac<sub>2</sub>O mixt. and kept 1 day to give 59.7% II diacetate, m. 171-2 degree.. A mixt. of 7.2 g. alpha., alpha., alpha.-trichloroacetanilide, 4.5 g. phenyl glycidyl ether, and 0.1 g. triethylenediamine was heated 2 hrs. at 100 degree. to give 3-phenyl-5-phenoxyethyl-2-oxazolidone, m. 138-9 degree.. Similarly from the trichloro and trifluoro derivs. the following III were prepd. (R, R<sub>1</sub>, % yield, and m.p. given): Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 70, 198-9 degree.; Ph, p-MeOC<sub>6</sub>H<sub>4</sub>, 78, 144-6 degree.; Ph, p-ClC<sub>6</sub>H<sub>4</sub>, 75, 192-4 degree.; Ph, p-MeC<sub>6</sub>H<sub>4</sub>, 85, 197-8 degree.; Ph, p-tert-BuC<sub>6</sub>H<sub>4</sub>, 80, 138-40 degree.; Ph, o-MeC<sub>6</sub>H<sub>4</sub>, 73, 91-4 degree.; Ph, beta.-naphthyl, 88, 206-8 degree.; p-MeC<sub>6</sub>H<sub>4</sub>, Ph, 87, 149-51 degree..

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For diagram(s), see printed CA Issue.

I is synthesized by the reaction of RNHCOR' with II. In an example, 16.5 g. PhNHCO<sub>2</sub>Et is heated with 15.0 g. phenyl glycidyl ether 30 min. at 90 degree. in the presence of 0.5 g. NEt<sub>3</sub> to give I (R<sub>1</sub> = R<sub>2</sub> = Ph), m. 139-40 degree. (Me<sub>2</sub>CO), almost quant. Similarly are prepd. the following I (R<sub>1</sub>, R<sub>2</sub>, and m.p. given): p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, Ph, 162-3 degree. (Me<sub>2</sub>CO); p-ClC<sub>6</sub>H<sub>4</sub>, Ph, 158-60 degree. (Me<sub>2</sub>CO); p-EtOC<sub>6</sub>H<sub>4</sub>, Ph, 131-3 degree. (Me<sub>2</sub>CO); p-tolyl, Ph, 149-51 degree. (Me<sub>2</sub>CO); 2-pyridyl, Ph, 115-16 degree. (EtOH); 1-naphthyl, Ph, 129-30 degree. (EtOH); 2-naphthyl, Ph, 165-7 degree. (Me<sub>2</sub>CO); omicron-Cl-C<sub>6</sub>H<sub>4</sub>, Ph, 121.5-2.5 degree. (EtOH); omicron-tolyl, Ph, 115-16 degree. (EtOH); p-ACOC<sub>6</sub>H<sub>4</sub>, Ph, 195-7 degree. (Me<sub>2</sub>CO); p-EtOCOC<sub>6</sub>H<sub>4</sub>, Ph, 146-9 degree. (EtOH); Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 198-9 degree. (Me<sub>2</sub>CO); Ph, p-ACOC<sub>6</sub>H<sub>4</sub>, 144-6 degree.

(EtOH); Ph, p-ClC6H4, 192-4.degree. (Me2CO); Ph, p-tolyl, 197-8.degree. (Me2CO); Ph, p-Me3CC6H4, 138-40.degree. (EtOH); Ph, .omicronmicron-.tolyl, 91-4.degree. (EtOH); Ph, 1-naphthyl, 132-4.degree. (EtOH); Ph, 2-naphthyl, 206-8.degree. (Me2CO); p-ClC6H4, p-O2NC6H4, 168-70.degree. (EtOH); Ph, 2-naphthyl, p-ClC6H4, p-AcOC6H4, 142-4.degree. (EtOH); p-ClC6H4, p-ClC6H4, p-ClC6H4, 183-6.degree. (Me2CO); p-ClC6H4, p-tolyl, 205-7.degree. (Me2CO); p-ClC6H4, p-Me3CC6H4, 145-7.degree. (EtOH); p-ClC6H4, p-ClC6H4, .omicronmicron-.tolyl, 120-2.degree. (EtOH); p-ClC6H4, 1-naphthyl, 137-9.degree. (EtOH); p-ClC6H4, 2-naphthyl, 216-18.degree. (Me2CO); p-ClC6H4, p-O2NC6H4, 150-2.degree. (EtOH); p-ClC6H4, p-AcOC6H4, 119-21.degree. (EtOH); p-ClC6H4, p-ClC6H4, 174-6.degree. (Me2CO); p-ClC6H4, p-EtOC6H4, p-tolyl, 181-3.degree. (Me2CO); p-EtOC6H4, p-Me3CC6H4, 125-7.degree. (EtOH); p-EtOC6H4, .omicronmicron-.tolyl, 111-13.degree. (EtOH); p-EtOC6H4, 1-naphthyl, 120-2.degree. (EtOH); p-EtOC6H4, 2-naphthyl, 196-7.degree. (Me2CO); p-tolyl, p-O2NC6H4, 170-2.degree. (Me2CO); p-tolyl, p-AcOC6H4, 136-8.degree. (EtOH); p-tolyl, p-ClC6H4, 199-201.degree. (Me2CO); p-tolyl, (EtOH-Me2CO); p-tolyl, p-ClC6H4, 151-3.degree. (EtOH); 1-naphthyl, 123-5.degree. (EtOH); .omicronmicron-.tolyl, 100-2.degree. (EtOH); p-tolyl, (Me2CO); 2-pyridyl, p-O2NC6H4, 197-9.degree. (Me2CO); 2-naphthyl, 196-8.degree. (Me2CO); 2-pyridyl, (EtOH); 2-pyridyl, p-ClC6H4, 181-3.degree. (Me2CO); 2-pyridyl, p-tolyl, 171-3.degree. (Me2CO); 2-pyridyl, p-Me3CC6H4, 112-14.degree. (EtOH); 2-pyridyl, .omicronmicron-.tolyl, 126-8.degree. (EtOH); 2-pyridyl, 1-naphthyl, 147-9.degree. (EtOH); 2-pyridyl, 2-naphthyl, 171-3.degree. (EtOH-Me2CO); 1-naphthyl, p-O2NC6H4, 179-81.degree. (Me2CO); 1-naphthyl, p-AcOC6H4, 126-8.degree. (EtOH); 1-naphthyl, p-ClC6H4, 144-6.degree. (EtOH); 1-naphthyl, p-tolyl, 146-8.degree. (EtOH); 1-naphthyl, p-Me3CC6H4, 148-50.degree. (EtOH-Me2CO); 1-naphthyl, .omicronmicron-.tolyl, 140-1.degree. (EtOH-Me2CO); 1-naphthyl, 1-naphthyl, 157-9.degree. (EtOH); 1-naphthyl, 2-naphthyl, 146-8.degree. (EtOH-Me2CO); 2-naphthyl, p-O2NC6H4, 223-5.degree. (Me2CO); 2-naphthyl, 146-8.degree. (EtOH-Me2CO); 2-naphthyl, p-tolyl, 214-16.degree. (Me2CO); 2-naphthyl, p-ClC6H4, 207-8.degree. (Me2CO); 2-naphthyl, (EtOH-Me2CO); 2-naphthyl, .omicronmicron-.tolyl, 145-7.degree. (EtOH-Me2CO); 2-naphthyl, 1-naphthyl, 138-40.degree. (EtOH-Me2CO); 2-naphthyl, 2-naphthyl, 201-3.degree. (Me2CO); .omicronmicron-.ClC6H4, p-ClC6H4, 124-5.degree. (EtOH); .omicronmicron-.ClC6H4, p-tolyl, 103-4.degree. (EtOH); .omicronmicron-.ClC6H4, p-Me3CC6H4, 111-12.degree. (EtOH); .omicronmicron-.tolyl, p-ClC6H4, 90-2.degree. (EtOH); .omicronmicron-.tolyl, p-tolyl, 84-5.degree. (EtOH); .omicronmicron-.tolyl, p-Me3CC6H4, 101-2.degree. (EtOH); .omicronmicron-.tolyl, 2-naphthyl, 129-30.degree. (EtOH).

=> d l5 1-14 ibib abs hitstr

MISSING OPERATOR D L5

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> d l5 1-14 ibib abs hitstr

L5 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2003:673836 CAPLUS  
DOCUMENT NUMBER: 139:214121  
TITLE: Preparation of ester group-containing ethers, sulfides, or amines

INVENTOR(S): Suzuki, Takashi; Kimura, Kazuhiko; Watanabe, Ryuzo  
PATENT ASSIGNEE(S): Konica Co., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.  
CODEN: JXXKXAF

DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE  
JP 2003238483 A2 20030827 JP 2002-33867 20020212  
PRIORITY APPLN. INFO.: MAPPAT 139-214121 20020212  
OTHER SOURCE(S):

AB RAY(CR1R2)m(L1)RCO2R6 (I; R1, R2 = H, alkyl, cycloalkyl, aryl; R4 = alkyl, cycloalkyl, aryl, heterocyclyl; R6 = alkyl, cycloalkyl, aryl; Y = O, S, NR7; L1 = O, S, CO, SO2, NR8, alkylene, arylene; R7 = H, alkyl, cycloalkyl, aryl, heterocyclyl, sulfonyl; R8 = H, alkyl, cycloalkyl, aryl, heterocyclyl, acyl, sulfonyl, alkoxy, carbonyl, aryloxy, carbonyl, carbamoyl, sulfamoyl; m = 1-10; n = 0-10; R7 may be bonded to R4 forming a ring) are prepd. by reacting X(CR1R2)m(L1)RCO2R3 (II; R1, R2, L1, m, n = same as above; R3 = alkyl, cycloalkyl, aryl; X = halo) with R4YH (R4, Y = same as above) in R5OH (R5 = alkyl, cycloalkyl, R5 = noted, R3). Use of R5OH which is different from alc. components of II, i.e. R3OH, reduces formation of carboxylic acids formed upon hydrolysis of products I. The reaction may be carried out in the presence of anhyd. metal salts capable of releasing water of crystn. upon heating. 2,5-BuO(tert-C8H17)C6H3SH was added to EtOH, mixed with Br(CH2)5CO2C8H17 at room temp., and the mixt. was heated under reflux for 3 h to give a product contg. 2,5-BuO(tert-C8H17)C6H3S(CH2)5CO2ZET 6.1, 2,5-BuO(tert-C8H17)C6H3S(CH2)5CO2H (IV, impurity 1.6%, vs. 92.2% III and 3.6% IV for a control using octanol instead of EtOH as a solvent.

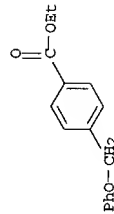
IT 56442-41-2P 124397-37-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of ester group-contg. (thio)ethers or amines from haloesters and alcs., thioals, or amines in alcs. different from alc. components of the esters)

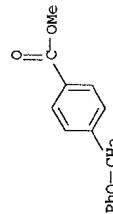
RN 56442-41-2 CAPLUS

CN Benzoic acid, 4-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 124397-37-1 CAPLUS

CN Benzoic acid, 4-(phenoxymethyl)-, methyl ester (9CI) (CA INDEX NAME)



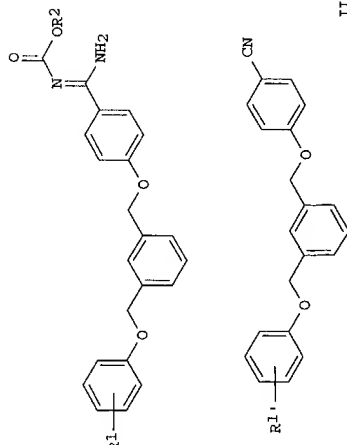
L5 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2001:523500 CAPLUS  
DOCUMENT NUMBER: 135:107153

TITLE: Procedure for the production of aryl iminomethyl carbanic acid esters  
INVENTOR(S): Brandenburg, Joerg; Soyka, Rainer; Schmid, Rolf; Anderskewitz, Ralf; Bauer, Rolf; Hamm, Rainer; Kroeber, Jutta

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany  
SOURCE: Ger. Offen., 12 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10000907	A1	20010719	DE 2000-10000907	20000112
US 2001009958	A1	20010726	US 2001-757253	20010109
US 6417382	B2	20040709		
WO 2001051457	A2	20010719	WO 2001-EP262	20010111
WO 2001051457	A3	20020117		
W: AE, AU, BG, BR, CA, CN, CZ, EE, HU, ID, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
BR 2001007551	A	20021008	BR 2001-7551	20010111
EP 1250318	A2	20021023	EP 2001-942357	20010111
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, IR				
JP 2003523328	T2	20030805	JP 2001-551839	20010111
EE 200200392	A	20031015	EE 2002-392	20010111
US 2002137963	A1	20020926	US 2002-138955	20020505
NO 200203348	A	20020711	NO 2002-3348	20020711
BG 106916	A	20030430	BG 2002-106916	20020712
DE 2000-10000907 A 20000112				
US 2000-177378P P 20000124				
US 2001-757253 A1 20010109				
WO 2001-EP262 W 20010111				
CASREACT 135-107153; MARPAT 135-107153				

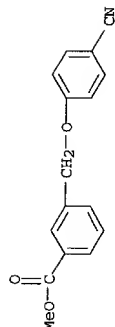
OTHER SOURCE(S):  
GI



AB The title compds. [I; C1-3 alkyl, cyclopentyl, cyclohexyl, Ph, PhCH<sub>2</sub>, (un)substituted C(CH<sub>3</sub>)<sub>2</sub>Ph; R<sub>2</sub> = C1-3 alkyl, PhCH<sub>2</sub>] [e.g., Et [4-[3-[4-[1-(4-hydroxyphenyl)-1-methylethyl]phenoxy]methyl]benzyl]oxy]phenyl

[iminomethyl]carbamate] are prepd. in high yield by the reaction of benzonitriles (II) in an arom. or ether solvent with lithium bis(trimethylsilyl)amide, sodium bis(trimethylsilyl)amide, or potassium bis(trimethylsilyl)amide, followed by reaction of the intermediate with carbonate ester halide R<sub>2</sub>O<sub>2</sub>CX (X = Cl, Br, OR<sub>2</sub>) followed by treatment with aq. HCl to give a hydrochloride salt of I.  
IT 167569-28-02, Methyl 3-(4-cyanophenoxy)methylbenzoate  
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

Procedure for the prodn. of aryl iminomethyl carbanic acid esters)  
RN 167569-28-0 CAPLUS  
CN Benzoic acid, 3-[(4-cyanophenoxy)methyl]-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2000:277952 CAPLUS  
DOCUMENT NUMBER: 132:278989  
TITLE: Method for drying water- and/or solvent-wet 2-(phenoxy)methyl benzoic acids  
INVENTOR(S): Isak, Heinz; Lambert, Martin  
PATENT ASSIGNEE(S): BASF A.-G., Germany  
SOURCE: PCT Int. Appl., 39 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

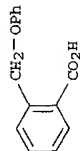
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000023413	A1	20000427	WO 1999-EP7826	19991015
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19848200	A1	20000427	DE 1998-19848200	19981020
EP 1123266	A1	20010816	EP 1999-950745	19991015
EP 1123266	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT, IE, FI				
JP 2002527499	T2	20020827	JP 2000-577141	19991015
AT 241583	E	20030615	AT 1999-950745	19991015
PRIORITY APPLN. INFO.: DE 1998-19848200 A 19981020				
OTHER SOURCE(S): MARPAT 132:278989				
GI				

catalytic amt. of DMF, and without isolation of acid chlorides  
cyclocondensation with catalytic amt. of Lewis acids. 3-FC64OH was  
treated with phthalide in the presence of MeONa at 155-160 degree for 4 h  
to give 78% 2-(3-fluorophenoxymethyl)benzoic acid, which was chlorinated  
with SOCl2 in the presence of DMF at 80 degree for 2 h and  
cyclocondensed using AlCl3 at 20 degree for 2 h to give 88%  
3-fluoro-6,11-dihydrodibenz[b,e]oxepin-11-one.

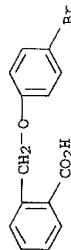
IT 724-98-1P, 2-phenoxymethylbenzoic acid 728-96-1P

RL: IMF (Industrial manufacture); RCT (Reactant or reagent)  
preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of dihydrodibenzoxepinones by ring opening of phthalides with  
phenols, chlorination, and cyclocondensation)

RN 724-98-1 CAPLUS  
CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



RN 728-96-1 CAPLUS  
CN Benzoic acid, 2-[(4-bromophenoxy)methyl]- (9CI) (CA INDEX NAME)



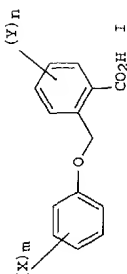
L5 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1993:38276 CAPLUS  
DOCUMENT NUMBER: 118:38276  
TITLE:  
Open-chain nitrogen compounds. Part XV. A kinetic  
study of the hydrolysis of 1-aryl-3-[(aryloxy)methyl]-  
3-methyltriazenes and related triazenes

AUTHOR(S):  
Vaughan, Keith; Hooper, Donald L.; Merrin, Marcus P.  
CORPORATE SOURCE:  
Saint Mary's Univ., Halifax, NS, B3H 3C3, Can.  
SOURCE:  
Canadian Journal of Chemistry (1992), 70(8), 2224-33  
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE:  
Journal

LANGUAGE:  
English

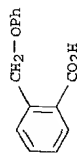
AB The kinetics of hydrolysis of 4-MeOCOC6H4N-NMeCH2OC6H4R-4 (I; R = OMe, Me, H, Cl, Br, CO2Me, CN, NO2) were studied over the pH range 2-7.5. I decomd. more slowly at pH 7.5 than the (hydroxymethyl)triazenes, ArN-NMeCH2OH; the hydrolysis was favored by electron-withdrawing R. A mixed isopropanol/buffer system was used to improve soly. of I. Lowering the pH increased the rate of hydrolysis, and under strongly acidic conditions an electron-withdrawing R substituent actually slowed the reaction. A Hammett plot of the pseudo-first-order rate const., Kobs, was curved, indicating that two or more mechanisms operated simultaneously and that the contribution of each was substituent-dependent. A plot of Kobs vs. [buffer] was linear; the slope of the plot afforded the rate const., kb, for the buffer-catalyzed reaction for each substituent. A Hammett plot of kb vs. sigma was linear with rho = +0.55, suggesting that the buffer-catalyzed reaction involved nucleophilic displacement of the phenoxy group by the buffer anion. Further anal. afforded the specific acid-catalyzed rate constants, kH+, for each substituent; this component of the reaction has a neg. rho, consistent with a mechanism involving protonation at the ether oxygen. The postulation that specific acid catalysis is a component of the reaction mechanism was confirmed by the



AB 2-(phenoxymethyl)benzoic acids (I; X, Y = halogen, C-org. radical; m = 0-5; n = 0-4) [e.g., 2-[(2-methylphenoxy)methyl]benzoic acid], wet with water and/or a solvent [e.g., methanol], are efficiently dried at 1-25 degree above the m.p.

IT 724-98-1DP, 2-(phenoxymethyl)benzoic acid, derivs.  
RL: PUR (Purification or recovery); PREP (Preparation)  
(method for drying water- and/or solvent-wet  
2-(phenoxymethyl)benzoic acids)

RN 724-98-1 CAPLUS  
CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1997:702036 CAPLUS  
DOCUMENT NUMBER: 127:358800

TITLE:  
Preparation of 6,11-dihydrodibenz[b,e]oxepin-11-ones  
INVENTOR(S):  
Nishizawa, Susumu; Ueno, Hiroki  
PATENT ASSIGNEE(S):  
Sumika Fine Chemicals Co., Ltd., Japan  
SOURCE:  
Jpn. Kokai Tokkyo Koho, 9 pp.  
CODEN: JKXXAF

DOCUMENT TYPE:  
Patent

LANGUAGE:  
Japanese

FAMILY ACC. NUM. COUNT:  
1

PATENT INFORMATION:

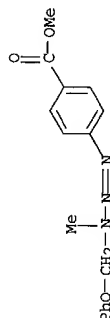
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09278774	A2	19971028	JP 1996-111952	19960408
PRIORITY APPLN. INFO.:			JP 1996-111952	19960408
OTHER SOURCE(S):			CASREACT 127:358800; MARPAT 127:358800	

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Oxepinones I (R1 = H, Me; R2 = H, Cl-4 alkyl, OH, F, Cl, Br, nitrile, NO2, Cl-3 dialkylamino, Cl-4 alkoxy, etc.; R3 = H, F, Cl, Br, nitrile, NO2, Cl-4 alkyl, Cl-4 alkoxy, Cl-4 alkoxy-carbonyl; n = 0-4) are prepd. by reaction of phenols II (R1, R2, n = same as I) with phthalides III (R3 = same as I) in the presence of MeONa at 150-180 degree, chlorination of IV (R1, R2, R3, n = same as I) with SOCl2 in PhNO2 in the presence of



observation of a solvent deuterium isotope effect, 2.28 > KH/RD  
> 1.60. Only I (R = CN, NO2) showed any spontaneous decompn.  
IT 142273-09-4 CAPLUS  
RU: PEP (Physical, engineering or chemical process); PREP (Properties); RCT  
(Reactant); PROC (Process); RACT (Reactant or reagent)  
(hydrolysis of, kinetics of)  
RN 142273-09-4 CAPLUS  
CN Benzoic acid, 4-[3-methyl-3-(phenoxymethyl)-1-triazenyl]-, methyl ester  
(9CI) (CA INDEX NAME)



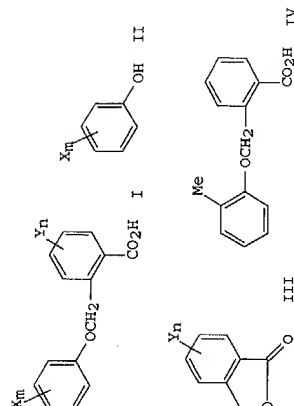
L5 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1992-570979 CAPLUS  
DOCUMENT NUMBER: 117-170979  
TITLE: Preparation of 2-(phenoxymethyl)benzoic acids from  
peroxides and phthalides  
INVENTOR(S): Wolf, Bernd; Benoit, Remy; Sauter, Hubert; Wingert,  
Horst; Hepp, Michael; Kuekenhoeher, Thomas;  
Grammenos, Nassilios  
PATENT ASSIGNEE(S): BASF A.-G., Germany  
SOURCE: Ger. Offen., 7 pp.  
CODEN: GWXXEX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 6  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4042283	A1	19920702	DE 1990-4042283	19901231
EP 493711	A1	19920708	EP 1991-121148	19911210
EP 493711	B1	19960925		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
EP 712835	A2	19960522	EP 1996-101025	19911210
EP 712835	A3	19960605		
EP 712835	B1	19970820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
EP 712833	A2	19960522	EP 1996-101038	19911210
EP 712833	A3	19960605		
EP 712833	B1	19970903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
EP 718279	A1	19960626	EP 1996-101039	19911210
EP 718279	B1	19970924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
AT 143356	E	19961015	AT 1991-121148	19911210
ES 2091278	T3	19961015	ES 1991-121148	19911210
AT 157079	E	19970915	AT 1996-101025	19911210
AT 157643	E	19970915	AT 1996-101038	19911210
AT 158569	E	19971015	AT 1996-101039	19911210
ES 2105903	T3	19971016	ES 1996-101025	19911210
ES 2105904	T3	19971016	ES 1996-101038	19911210
US 2107923	T3	19971201	US 1996-101039	19911210
US 5221762	A	19930622	US 1991-806295	19911210
IL 100387	A1	19970610	IL 1991-100387	19911216
IL 116442	A1	19970610	IL 1991-116442	19911216

IL 116443	A1	19970610	IL 1991-116443	19911216
JP 04295454	A2	19921020	JP 1991-338127	19911220
JP 334263	B2	20021111		
JP 2000256273	A2	20000919	JP 2000-100964	19911220
JP 3378555	B2	20030217		
AU 9190082	A1	19920702	AU 1991-90082	19911224
AU 641579	B2	19930923		
CA 2058553	AA	19920701	CA 1991-2058553	19911230
HU 61284	A2	19921228	HU 1991-4162	19911230
HU 209283	B	19940428		
JP 2002356468	A2	20021213	JP 2002-116019	20020418
JP 3378576	B2	20030217		

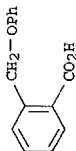
PRIORITY APPLN. INFO.:  
DE 1990-4042271 A 19901231  
DE 1990-4042272 A 19901231  
DE 1990-4042273 A 19901231  
DE 1990-4042280 A 19901231  
DE 1990-4042282 A 19901231  
DE 1990-4042283 A 19901231  
EP 1991-121148 A3 19911210  
IL 1991-100387 A3 19911216  
JP 1991-338127 A3 19911220  
CASREACT 117:170979; MARPAT 117:170979

OTHER SOURCE(S):  
GI



AB Title compds. (I; X, Y = halo, alkyl, alkoxy, CF3; m = 0-4; n = 0-3), were  
prepd. by a) conversion of phenol II to a phenolate by treatment with  
base, b) mixing the phenolate soln. with lactone III, c) distn. of  
solvent and heating of the resultant mixt. to 50-250.degree..  
Thus, o-cresol was stirred with NaOMe in MeOH at 50.degree.; phthalide was  
added and solvent was distd. off. The residue was heated at  
200.degree. to give 89% title compd. IV.  
IT 724-98-IP  
RL: SEN (Synthetic preparation); PREP (Preparation)  
(prepn. of, from phenol and phthalide)  
RN 724-98-1 CAPLUS  
CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

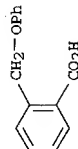
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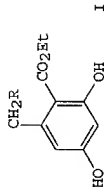
L5 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1986-2071175 CAPLUS  
 DOCUMENT NUMBER: 104:2071175  
 TITLE: 6,11-Dihydrodibenz[b,e]oxepin-11-one  
 INVENTOR(S): Fuchs, Oszkar; Nemes, Andras; Toldy, Lajos; Kaeztreiner, Endre; Lazar, Arpad; Somogyi, Tibor; Balogh, Tibor  
 PATENT ASSIGNEE(S): Gyogyszerkutato Intezet, Hung.  
 SOURCE: Hung. Teljes, 9 pp.  
 CODEN: HUXXB  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Hungarian  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 34969	O	19850528	HU 1983-2142	19830616
HU 192812	B	19870728	HU 1983-2142	19830616

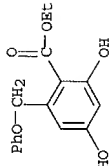
OTHER SOURCE(S): CASREACT 104:207175  
 AB 6,11-Dihydrodibenz[b,e]oxepin-11-one (I) is prepd. by the cyclization of 2-phOCH2C6H4COCl (II) (pred. from the parent acid and SOCl2) in an arom. solvent at 60-120 degree. in the presence of Fe or alk. earth metal or oxide. Thus II (freshly prepd. from 6.84 kg the parent acid) in 20 L benzene was heated with 70 g freshly-reduced Fe to give 5.25 kg I. I is the starting material in the synthesis of doxepin.  
 IT 724-98-1  
 RL: PROC (Process)  
 (conversion of, into acid chloride)  
 RN 724-98-1 CAPLUS  
 CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1979:474309 CAPLUS  
 DOCUMENT NUMBER: 91:74309  
 TITLE: Studies on ketene and its derivatives. Part 89. Ethyl 4-substituted acetoacetates: Synthesis and reaction with diketene  
 Kato, Tetsuzo; Sato, Masayuki; Kimura, Hitochi  
 Pharm. Inst., Tohoku Univ., Sendai, Japan  
 Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1979), (2), 529-32  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English



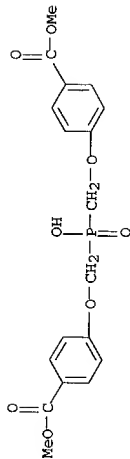
AB The benzoates I (R = Br, OEt, OPh, OCH2Ph, SPh, OAc) were prepd. (8-33%) by reaction of diketene with RCH2COCH2CO2Et (II). II (R = OEt, OPh, OCH2Ph, SPh, OAc) were obtained (44-70%) from II (R = Br) by reaction with NaR.  
 IT 71027-67-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 71027-67-3 CAPLUS  
 CN Benzoic acid, 2,4-dihydroxy-6-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1974:146640 CAPLUS  
 DOCUMENT NUMBER: 80:146640  
 TITLE: Synthesis of a copolymer from bis(p-carbomethoxy)phenoxymethylphosphinic acid, dimethyl terephthalate, or dimethyl sebacate and ethylene glycol  
 Borisov, G.; Devedzhiev, I.  
 Inst. Org. Chem., Sofia, Bulg.  
 Izvestiya na Otdelenieto za Khimicheski Nauki (Bulgarska Akademiya na Naukite) (1972), 5(4), 553-9  
 CODEN: IOKNA5; ISSN: 0525-0889  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Bulgarian  
 AB Bis(p-(methoxycarbonyl)phenoxymethyl)phosphinic acid (I) [ 47554-39-2] improved the thermal stability and fire resistance of poly(ethylene sebacate) [25034-96-2] and poly(ethylene terephthalate) [25038-59-9] copolymers. The polycondensation was carried out in the melt and the copolymers were sol. in basic solvents.  
 IT 51749-75-8 51749-76-9  
 RL: USES (Uses)  
 (fire-resistant thermally-stable)  
 RN 51749-75-8 CAPLUS  
 CN Decanedioic acid, dimethyl ester, polymer with dimethyl 4,4'-[phosphinicobis(methyleneoxy)]bis(benzoate) and 1,2-ethanediol (9CI) (CA INDEX NAME)

CM 1  
 CRN 47554-39-2

CMF C18 H19 O8 P



CM 2

CRN 107-21-1

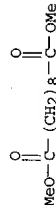
CMF C2 H6 O2

HO-CH<sub>2</sub>-CH<sub>2</sub>-OH

CM 3

CRN 106-79-6

CMF C12 H22 O4



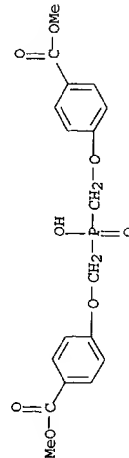
RN 51749-76-9 CAPLUS

CN 1,4-Benzenedicarboxylic acid, dimethyl ester, polymer with dimethyl 4,4'-[phosphinobis(methyleneoxy)]bis(benzoate) and 1,2-ethanediol (9CI) (CA INDEX NAME)

CM 1

CRN 47554-39-2

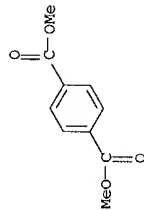
CMF C18 H19 O8 P



CM 2

CRN 120-61-6

CMF C10 H10 O4



CM 3

CRN 107-21-1

CMF C2 H6 O2

HO-CH<sub>2</sub>-CH<sub>2</sub>-OH

L5 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1973:44024 CAPLUS

DOCUMENT NUMBER: 78:44024

TITLE: Obtaining bis(p-carboxyphenoxyethyl)phosphinic acid, its esters, and polyesters

AUTHOR(S): Borisov, G.; Devedzhiev, I.

CORPORATE SOURCE: Inst. Org. Chem., Sofia, Bulg.

SOURCE: Doklady Bolgarskoi Akademii Nauk (1972), 25(6), 759-62

CODEN: DEANAD; ISSN: 0366-8681

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Bis(p-carboxyphenoxyethyl)phosphinic acid (I) [37394-15-3] was

prepd. by treatment of p-HOC6H4CO2Me with Na and (ClCH2)2P(O)OH followed by sapon. with alc. K peroxide; I was copolymd. with each of 5 diols to give polyesters which were fire resistant and self-extinguishing. The polyesters had softening temps. sim. 300 deg. were insol. in ordinary org. solvents but sol. in org. and inorg. bases, and were capable of being drawn into fibers.

IT 47554-39-2P

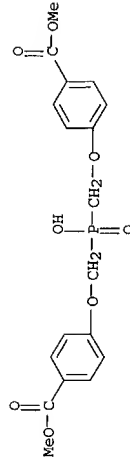
RL: SEN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 47554-39-2 CAPLUS

CN Benzoic acid, 4,4'-[phosphinobis(methyleneoxy)]bis-, dimethyl ester

(9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1971:105074 CAPLUS

DOCUMENT NUMBER: 74:105074

TITLE: Substituent effects in infrared spectroscopy. I. The

O-H stretching frequencies in monomeric benzoic acids

Exner, Otto; Svatek, E.

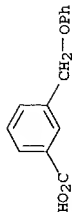
CORPORATE SOURCE: Cesk. Akad. Ved, Prague, Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (1971), 36(2), 534-43  
CODEN: CCCCAC; ISSN: 0010-0765

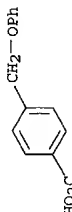
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The O-H stretching frequencies of 60 meta- and para-substituted benzoic acids were measured in dil. CCl<sub>4</sub> soln. The IR values were correlated by the Hammett equation with normal  $\sigma$ -sigma, const. and slope  $\rho$ -rho = -11.7 cm<sup>-1</sup> on the one hand, and by the equation  $\nu$ - $\nu$  = 1.14 ( $\nu$ - $\nu$ ) on the other hand, where the frequency  $\nu$  refers to the unsubstituted compd. The validity of the latter for substituents without an  $\alpha$ -alpha lone electron pair was confirmed even in IR spectroscopy. Somewhat lesser accuracy of the Hammett correlation is probably due to a different solvent than used in detg. the  $\sigma$ -sigma, const.; deviations of a systematic character were not obsd.

IT 31719-75-2 31719-76-3  
RL: PRP (Properties) (spectrum of, IR)  
RN 31719-75-2 CAPLUS  
CN Benzoic acid, 3-(phenoxymethyl)- (9CI) (CA INDEX NAME)



RN 31719-76-3 CAPLUS  
CN Benzoic acid, 4-(phenoxymethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1970:121634 CAPLUS  
DOCUMENT NUMBER: 72:121634

TITLE: Syntheses based on tetramethyldiethylenetriamine chloride. Some transformations of tris(chloromethyl)phosphine and methyldibis(chloromethyl)phosphine oxide  
Tsvetkov, E. N.; Borisov, G.; Siliviev, Kh.; Mavannaya, R. A.; Kabachnik, M. I.  
Inst. Elementoorg. Soedin., Moscow, USSR  
Zhurnal Obshchei Khimii (1970), 40(2), 285-91  
CODEN: ZOKH44; ISSN: 0044-460X

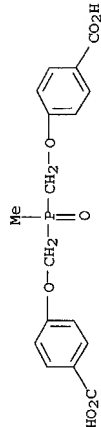
AUTHOR(S): Russian  
CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR  
SOURCE: Zhurnal Obshchei Khimii (1970), 40(2), 285-91

DOCUMENT TYPE: Journal  
LANGUAGE: Russian

AB Addn. of 350 g (HOCH<sub>2</sub>)<sub>4</sub>PCl<sub>2</sub> to 1680 g PCl<sub>5</sub> in 2 l. CCl<sub>4</sub> at reflux and heating 4 hr gave 97% (ClCH<sub>2</sub>)<sub>4</sub>PCl<sub>2</sub> (I), m. 198-9.degree. I (200 g) treated with 60-7 g NaOH in 300 ml H<sub>2</sub>O at 10-15.degree. in 400 ml H<sub>2</sub>O-400 ml CHCl<sub>3</sub> until alk. to phenolphthalein, gave 81.5% (ClCH<sub>2</sub>)<sub>3</sub>PCl<sub>2</sub> (II), b<sub>2</sub> 56-7.degree., d<sub>20</sub> 1.4204, n<sub>D</sub> 20D 1.5330, which on standing deposited a flaky colorless solid of undetd. compn.; during evapn. of the solvent from II the temp. must be held under 90.degree. as explosions occurred at 100.degree. or higher. II and 24% NaOH at 10-20.degree., then at reflux 3 hr until homogeneous gave MeP(O)(CH<sub>2</sub>Cl)<sub>2</sub> (III), b<sub>7</sub> 149-50.degree., m. 49-50.degree. III also formed after similar heating of II with H<sub>2</sub>O alone. Heated with NaOAc-ACOH 6 hr at 200.degree. III gave the diacetate, b<sub>5</sub> 16 3-4.degree., 1.2326, 1.4670, also prepd. from II and ACOH-ACONA 10

hr at 150.degree.. Heating II with EtSH-EtSNa 9 hr at 130.degree. in Et<sub>2</sub>O in an autoclave gave 84% (EtSCH<sub>2</sub>)<sub>3</sub>P, b<sub>2</sub> 137-8.degree., 1.0749, 1.5665. MeP(O)(CH<sub>2</sub>Cl)<sub>2</sub> (IV) and Et<sub>2</sub>NH in 15 hr at 125.degree. gave 49% MeP(O)(CH<sub>2</sub>NEt)<sub>2</sub>, b<sub>2</sub> cntdot. 5 118-19.degree., 0.9391, 1.4681. Heating 3 g IV and 10 g Ph<sub>3</sub>P in Me<sub>2</sub>NCHO 12 hr at 150-60.degree. gave 0 n addn. of Me<sub>2</sub>CO reaction product of 1.37 g Na and 10 ml MeOCH<sub>2</sub>CH<sub>2</sub>OH in MePh gave in 6 hr refluxing 53.5% MeP(O)(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub>, b<sub>5</sub> 185-6.degree., 1.1117, 1.4625. Similarly was prepd. 52% MeP(O)(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OBu)<sub>2</sub>, b<sub>5</sub> 210-11.5.degree., 1.0082, 1.4547. Ph<sub>3</sub>Na similarly gave 83% MeP(O)(CH<sub>2</sub>OPh)<sub>2</sub>, m. 96-7.degree.. Similarly was prepd. 80% p-tolyl analog, m. 122-4.degree.; 79% p-nitrophenyl analog, m. 169-70.degree.; m-nitrophenyl analog, m. 90-1.degree.; p-carbomethoxyphenyl analog, m. 133-5.degree.; p-carboxyphenyl analog, m. 295-6.degree.; m-isomer, m. 142-3.degree..

IT 26344-37-6P  
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)  
RN 26344-37-6 CAPLUS  
CN Benzoic acid, 4,4'-[(methylphosphinylidene)bis(methyleneoxy)]bis- (9CI) (CA INDEX NAME)



L5 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1966:4124 CAPLUS  
DOCUMENT NUMBER: 64:4124  
ORIGINAL REFERENCE NO.: 64:719c-e, 720a-b

TITLE: Dibenzo[b,e]oxepin-11-ones  
INVENTOR(S): Bloom, B. M.; Tretter, J. R.  
PATENT ASSIGNEE(S): Chas. Pfizer & Co. Inc.  
SOURCE: 45 PP.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 641498			BE	
GB 1018995		19640618	GB	

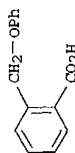
PRIORITY APPLN. INFO.: US 19620313  
AB The title compds. (I) were prepd. from the corresponding dibenzoxepin-11-one (II) and RRINCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>MgCl (III) and the resulting carbinol (IV) was salted to I with mineral acids. Some salts of I were separated as dehydrates of the cis and trans isomer by fractional crystn. The given synthesis affords a mixt. of 18% cis and 82% trans I. I are used as drugs in mental depression. The cis isomer is much more active than the trans one. Omicron-BrCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Et (27.5 g.) is added to a soln. of 7.05 g. PhOH and 3 g. NaOH in 50 ml. H<sub>2</sub>O and the mixt. stirred at 100.degree. for 5 hrs. to give 10.22 g. Et 2-phenoxymethylbenzoate (V), b<sub>5</sub> 130-40.degree., V (10 g.) is added to a soln. of 100 ml. 10% 0.5 NaOH and 50 ml. EtOH and the mixt. refluxed 65 hrs. to give 8.9 g. 2-phenoxymethylbenzoic acid (VI), m. 125.5-26.5.degree., VI (15 g.) is added in 30 min. to 60 ml. (CF<sub>3</sub>CO)<sub>2</sub>O and the mixt. kept 4 hrs. at room temp. to give 10.5 g. II (X = Y = H), m. 70.5-1.5.degree.. To a soln. of III (R = R<sub>1</sub> = Me) in 200 ml. Et<sub>2</sub>O prepd. from 11.5 g. Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl and 2.28 g. Mg, a 10% ethereal soln. of II (X = Y = H) is added in 1 hr. and

the mixt. refluxed 20 hrs. to give 10 g. IV (X = Y = H, R = R1 = Me) (VII), m. 121-3 degree. VII (4.1 g.) in 100 ml. N HCl is refluxed 2 hrs. to give 3.08 g. I (X = Y = H, R = R1 = Me), b.p. 260-70 degree. HCl salt (Vila) m. 188-9 degree. VII (10.4 g.) in 125 ml. C6H6 is added in 3 hrs. to a soln. of 6 g. BrCN in 50 ml. C6H6. After 30 min. the solvent is evapd. at 15 mm. and 50 ml. C6H6 added to the residue; the soln. is washed with 50 ml. H2O, the solvent distd., 150 ml. 10% NaOH and 75 ml. EtOH are added to the residue, and the mixt. is refluxed 44 hrs. to give I (X = Y = H, R = H, R1 = Me) (VIII) as HCl salt, m. 241-2 degree. The following compds. are similarly prepd.: II (X = H, Y = 2-MeNSO2), 11-allyl-dibenz[e]oxepin-11-ol, III HCl (X = H, Y = 2-MeNSO2, R = H, R1 = Me), m. 199-201 degree. II (X = H, Y = F3C), m. 108.5-9.5 degree. VIIa HCl (5 g.) is converted to the free base and then to a maleate, m. 168-9 degree. Several crystals, from EtOH give the trans salt, m. 172-3 degree. The cis hydrochloride m. 209-10.5 degree. Similarly is prepd. cis-VIII HCl, m. 225-6.5 degree., which with HCHO and HCO2H gives cis-VIIa HCl. Heating 50 mg. trans-VIIa HCl 0.25 hr. on a steam bath with 5 ml. N HCl gives a mixt. of the cis and trans isomers.

IT 724-98-1, o-Toluic acid, alpha-phenoxy- 4504-85-2, (prepn. of)

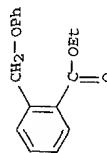
RN 724-98-1 CAPLUS

CN Benzoic acid, 2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



RN 4504-85-2 CAPLUS

CN Benzoic acid, 2-(phenoxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)



15 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1963:32717 CAPLUS

DOCUMENT NUMBER: 58:32717

ORIGINAL REFERENCE NO.: 58:5468d-h, 5469a-b

TITLE: Quantitative evaluation of the inductive effect

AUTHOR(S): Exner, O.; Jonas, J.

CORPORATE SOURCE: Ustav Org. Chemie Csl. Akad. Ved, Prague

SOURCE: Collection of Czechoslovak Chemical Communications (1962), 27, 02296-306

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

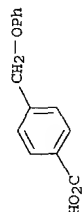
AB The relative pK' values obtained by measuring the disocn. consts. of p-toluic acids, substituted in the Me group, in 50% (by vol.) aq. EtOH (I) and 80% (by wt.) Methyl Cellosolve (II), are considered as a measure of the inductive effect of the substituents. From the results it follows that the transmission of the inductive effect takes place predominantly along the .delta.-bonds (and not space). Refluxing p-ClCH2C6H4CN (IIa) along the azetropic HBr 12 hrs. gave 62% p-BrCH2C6H4CO2H, m. 229 degree.

(EtOH), also formed in 90% yield by refluxing p-HOCH2C6H4CO2Me with the same reagent. p-ClCH2C6H4CO2H (III) (1.71 g.) and 4 g. NaI refluxed 1 hr. in 30 ml. Me2CO, and the soln. evapd. to dryness in vacuo, the inorg. salts washed out with H2O, and the product washed with a dil. soln. of Na2S2O3 gave 66% p-ICH2C6H4CO2H, m. 235 degree. (EtOH). Refluxing 1.71 g. III with 0.46 g. Na in 30 ml. abs. MeOH 3 hrs., evapd. the MeOH in vacuo, and pptg. by HCl gave 70% p-MeOCH2C6H4CO2H, m. 108 degree. (CHCl3, petr. ether). Similar procedure with 1.71 g. III, 0.94 g. PhOH, and 0.46 g. Na in 30 ml. MeOH gave 55% p-PhOCH2C6H4CO2H, m. 216 degree. (dil. EtOH). Adding 0.8 ml. AcCl to 1.52 g. p-HOCH2C6H4CO2H in 5 ml. C5H5N, cooling the mixt. after 15 min., and pouring into dil. HCl gave 88% p-AC-CH2C6H4CO2H, m. 128 degree. (C6H6). p-PhCH2C6H4CO2H, prepd. from p-BrCH2C6H4CN (IV) and C6H6 in a 68% overall yield, m. 160 degree. (dil. EtOH). Partial hydrolysis of p-NCH2C6H4CO2H afforded 51% p-H2NCH2C6H4CO2H, m. 274 degree. (EtOH). Refluxing 1.71 g. III with 1 g. NaSCN in 30 ml. EtOH 3 hrs., evapd. the soln. to dryness in vacuo, eluting the salts with H2O, and reprecip. the crude product from 10% aq. KOH gave 80% p-NCSCH2C6H4CO2H, m. 172 degree. (EtOAc). Refluxing 1.61 g. p-BrCH2C6H4CO2H with 2.2 g. PhSO2Na in 25 ml. EtOH 8 hrs. Yielded 95% p-PhSO2CH2C6H4CO2H, m. 306 degree. (decompn.) (EtOH). Adding 4.9 g. IV to a mixt. of 8.2 g. Me2NH.HCl and 3.5 g. NaOH in 10 ml. H2O and 25 ml. EtOH, allowing the mixt. to stand overnight, refluxing 30 min., evapd. the EtOH, in vacuo, dissolving the residue in H2O, extg. the soln. with three 15-ml. portions CHCl3, evapd. the ext., refluxing the residue 3 hrs. with a soln. of 3 g. NaOH in 20 ml. 50% EtOH, acidifying the reaction mixt. with HCl, evapd. to dryness in vacuo, and extg. the residue with boiling EtOH gave 56% p-Me2NCH2C6H4CO2H.HCl, m. 256 degree. (EtOH). Allowing a mixt. of 3.03 g. IIa and 2.8 g. (CH2)6N4 in 50 ml. CHCl3 to stand 2 days at room temp., concg. the soln. to 10 ml. in vacuo, filtering off 4.11 g. of a salt, dissolving it in 20 ml. 1:2 HCl and EtOH, distg. to dryness in vacuo, and extg. the residue with Me2CO gave 52% p-H2NCH2C6H4CN.HCl, m. 269 degree. (EtOH). Hydrolysis by refluxing 16 hrs. with concd. HCl, followed by acetylation with AcCl in pyridine, gave 43% p-AC-NHCH2C6H4CO2H, m. 201 degree. (EtOH). The measurements of the apparent disocn. consts. were carried out using an electronic pH meter with a vibrating condenser and a cell having a glass electrode and calomel reference electrode. The substances in concns. of the order of 10-3M were titrated with aq. Me4OH. The apparent disocn. consts. (pK') in solvents I and II for the appropriate substituents in .alpha.-position of p-MeC6H4CO2H are for: H, 5.78, 6.82; Cl, 5.36, 6.45; Br, 5.36, 6.36; Iodine, 5.41, 6.41; Ph, 5.70, 6.73; CN, 5.28, 6.32; CONH2, 5.44, 6.69; OH, 5.56, 6.70; OMe, 5.50, 6.58; SCN, 5.43, 6.56; OAc, 5.46, 6.50; NHAc, 5.61, 6.68; NMe2.HCl, 4.67, --; SO3Na, 5.33, 6.46; and PhSO2, --, 6.36

IT 31719-76-3 p-Toluic acid, alpha-phenoxy- (ionization of)

RN 31719-76-3 CAPLUS

CN Benzoic acid, 4-(phenoxymethyl)- (9CI) (CA INDEX NAME)



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6 AUG 18 Data available for download as a PDF in RDISCLOSURE  
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NEWS 8 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation

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NEWS 15	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16	NOV 24	MSDS-COHS file reloaded
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NEWS 17 DEC 08 CABA reloaded with left truncation  
NEWS 18 DEC 08 IMS file names changed  
NEWS 19 DEC 09 Experimental property data collected by CAS now available in program

NEWS 20 DEC 09 STN Entry Date available for display in REGISTRY and CA/Caplus in REGISTRY

NEWS EXPRESS NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01C, CURRENT

MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
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antagonists

IN Cournoyer, Richard Leo; Keitz, Paul Francis; Lowrie, Lee Edwin, Jr.;  
Muehlhoff, Alexander Victor; O'Yang, Counde; Yasuda, Dennis Mitsugu  
PA F. Hoffmann-La Roche A.-G., Switz.  
SO PCT Int. Appl., 100 pp.  
DT Patent  
LA English  
FAN CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2001068591 A1 20010920 WO 2001-EP2597 20010308

W: BE, AL, AM, AT, AU, AZ, BA, BE, BG, BR, BY, CA, CH, CN, CO, CU,  
CZ, DE, DK, EG, ES, FI, FR, GB, GR, GM, HR, HU, ID, IL, IN,  
IS, JP, KE, KG, KP, KR, LR, LS, LT, LU, LV, MA, MD,  
MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,  
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BJ, CF, CG, CI, CM, GN, GW, ML, MR, NE, SN, TD, TG

BR 2001009235 A 20021217 BR 2001-9235 20010308

EP 1265853 A1 20021217 EP 2001-9235 20010308

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 200327368 T2 2001-567688 20010308

US 20010356100 A1 20011127 US 2001-810436 20010314

NO 2002094387 A 20021021 NO 2002-4387 20020913

US 2003220367 A1 20031127 US 2003-434809 20030509

PRAI US 2000-190129P P 200000316

US 2000-247129P P 20001110

WO 2001-EP2597 W 20010308

US 2001-810436 A3 20010314

OS MARPAT 135:257467

RE CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS ON STN  
DN 126:212048

TI Substituted aromatic compounds and their pharmaceutical use as inhibitors  
of TNF and PDE IV.

IN Aldous, David John; Smith, Graham Frank; Astles, Peter Charles; Pickett,  
Stephen Dennis; McLay, Iain McFarlane; Stuttle, Keith Alfred James;  
Ratcliffe, Andrew James; et al.

PA Rhone-Poulenc Rorer Limited, UK; Aldous, David John; Smith, Graham Frank;  
Astles, Peter Charles; Pickett, Stephen Dennis; McLay, Iain McFarlane  
SO PCT Int. Appl., 159 pp.  
CODEN: PIXXD2

DT Patent  
LA English  
FAN CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 9703967 A1 19970206 WO 1996-GB1746 19960722

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EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR,  
LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU,  
SD, SE

RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,  
IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM

AU 9665268 A1 19970218 AU 1996-65268 19960722

PRAI GB 1995-15058 A 19950722

GB 1995-15729 A 19950801

GB 1996-4531 A 19960302

US 1996-14212P P 19960327  
WO 1996-GB1746 W 19960722  
MARPAT 126:212048

OS ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS ON STN

LA ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS ON STN

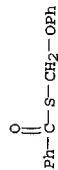
AB The title compds. (I-IV) are obtained from diazo ketones and ketenes.  
Thus, solns. of 6 g. BzCHN2 (V) and 8 g. Ph2C=CO (VI) in 20 ml. Et2O were  
combined under N, kept 1.5 hrs. at room temp., and evapd. to dryness. The  
residue was heated on a water bath until N evolution ceased and recrystd.  
from EtOH (C) to give 10.5 g. I (R = Ph), m. 120-1.degree.  
Similarly, reaction of 2.45 g. p-MeOC6H4COCHN2 and 2.7 g. VI in Et2O at  
room temp. gave 2.44 g. I (R = Ph, R1 = p-MeOC6H4), m. 164.degree.. A  
soln. of 2 g. p-O2NC6H4COCHN2 in abs. C6H6 was mixed with 2.04 g. VI and  
kept at room temp. overnight to give 1.56 g. I (R = Ph, R1 = p-O2NC6H4),  
m. 193-4.degree.. To a suspension of 13.1 g. V in 150 ml. xylene  
cooled to -45 to -50.degree. was added 25 ml. liquid ketene. After  
standing overnight (the temp. rose to 0.degree.), the soln. was filtered  
and evapd. in vacuo at 68.degree. to give 2.92 g. I (R = H, R1 = Et), m.  
92.degree.. Adding 14.25 g. VI to a cold soln. of 10 g.  
2-diazoacetylurea in Et2O, warming to 35% concg. after standing  
overnight, and recrystg. the ppt. from EtOH gave 4 g. I (R = Ph, R1 =  
2-furyl), m. 150-1.degree. A suspension of 12.3 g. 1-diazononadecan-2-  
one in 200 ml. abs. Et2O was mixed with a soln. of 7.75 g. VI in 80 ml.  
Et2O, kept 1 hr. at room temp., refluxed on a water bath, and kept again  
12 hrs. gave 5.33 g. I (R = Ph, R1 = p-MeOC6H4), m. 54.5.degree.. A  
soln. of 10 g. 1-diazoheptan-2-one in 100 ml. abs. PhMe was cooled to  
-60.degree. and mixed with 40 ml. ketene. Another 10 ml. ketene was added  
the next day. After a few days, the soln. was filtered, evapd. at 15 mm.,  
and the residue distd. at 1 mm. to give 4.9 g. I (R = H, R1 = Et), n.  
1.450, which was converted to homolevulinic acid, m. 38.degree., and then  
to n-hexanoic acid amide, m. 101.degree.. Similarly, a soln. of 9.9 g.  
.beta.-naphthoyldiazomethane in 150 ml. xylene was cooled to 60.degree.  
and treated with 40, 10, and 20 ml. ketene. Two days after the last  
addn. the soln. was filtered and cooled 1 hr. to -40.degree. to give 1.13  
g. I (R = H, R1 = 2-naphthyl), m. 142.degree.. This compd. was converted  
to 2-((beta.-naphthoyl)propionic acid, in. 175.degree., and the latter  
reduced to .gamma.-((2-naphthyl)butyric acid, m. 101.degree.. A soln. of  
2.72 g. p-IC6H4COCHN2 and 1.94 g. VI in 10 ml. abs. Et2O was kept at room  
temp. 3 hrs. and evapd. The residue was dissolved in 2 ml. PhMe, the  
soln. heated 20 min. on a water bath, refluxed 5 min., cooled, and the  
ppt. recrystd. from ligroine to give 2.45 g. I (R = Ph, R1 = p-IC6H4), m.  
156.degree.. A mixt. of 3.33 g. p-phenylbenzoyldiazomethane and 2.91 g. VI  
in 10 ml. abs. PhMe was kept 3 hrs. at room temp., heated 1.5 hrs. at  
100.degree., and, refluxed 5 min. to give 3.26 g. I (R = Ph, R1 =  
biphenyl), m. 195.degree. Solns. of 3.16 g. 2-diazoindan-1-one in 10  
ml. abs. Et2O and 3.88 g. VI in 10 ml. Et2O were combined under N and  
kept at room temp. overnight. After evapn. of the Et2O, the residue was



taken up in xylene, the soln. heated several hrs. on a water bath, kept at room temp. overnight, and evapd. in vacuo to give 0.45 g. II, m. 225.degree.. A suspension of 4.28 g. 1,4-bis(diazoacetyl)benzene and 7.76 g. VI in 30 ml. xylene was refluxed briefly and the clear soln. cooled to give 5 g. III [R = Ph, R1 = p-C6H4], m. 203.degree.. A mixt. of 0.55 g. 2,5-bis(diazoacetyl)thiophene (m. 193.degree.) in 2 ml. xylene and 0.97 g. VI in 3 ml. xylene was heated briefly on a water bath and kept at room temp. overnight. After several days, the ppt. was washed with very little xylene and petr. ether and recrystd. from EtOH to give 0.25 g. III [R = Ph, R1 = 2,5-thiophenediyl], m. 238.degree.. To a suspension of 13.72 g. 1,7-bisdiazoheptane-2,6-dione in 200 ml. xylene was added at -60.degree. 60 ml. ketene. After standing 3 days in dry ice-MeOH, the mixt. was worked up to give 6.28 g. III [R = H, R1 = (CH2)3], m. 104.5.degree.. Similarly, 3.18 g. 1,8-bisdiazoctane-2,7-dione in 70 ml. xylene and 10 ml. ketene gave 1.9 g. III [R = H, R1 = (CH2)4], m. 125.5.degree. (EtOH). A mixt. of 10 g. 1,9-bisdiazononane-2,8-dione in 100 ml. xylene and 50 ml. ketene was kept 2 days at -60.degree. and 2 days in a refrigerator to give 5.35 g. III [R = H, R1 = (CH2)5], m. 75.degree.. To a soln. of 6.2 g. 1,10-bisdiazoodecane-2,9-dione in 150 ml. xylene was added at -60.degree. 40 ml. ketene and the next day another 20 ml. After several days, the soln. was filtered, dild. with 3 vol. petr. ether, cooled to -18.degree., and the ppt. was crystd. from ligroine to give 2.21 g. III [R = H, R1 = (CH2)6], m. 105.degree.. A suspension of 5.64 g. 1,3,5-tris(diazoacetyl)benzene in 40 ml. xylene was treated with 11.64 g. VI, kept 35 min. at room temp., heated during 1 hr. from 60 to 90.degree., and refluxed 2-3 min. After 3 days at room temp., the ppt. was filtered to give 4.52 g. IV hydrate, m. 255-6.degree..

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L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS ON STN  
 IT 1955-50-6, Benzoic acid, thio-, S-phenoxyethyl ester  
 (prepn. of)  
 RN 1955-50-6 CAPLUS  
 CN Benzoic acid, thio-, S-(phenoxyethyl) ester (7CI, 8CI) (CA INDEX NAME)



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